



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:13 AM UTC

PDB ID : 6CI9 / pdb_00006ci9
Title : RMM microcompartment-associated aminopropanol dehydrogenase NADP + aminoacetone holo-structure
Authors : Mallette, E.; Kimber, M.S.
Deposited on : 2018-02-23
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

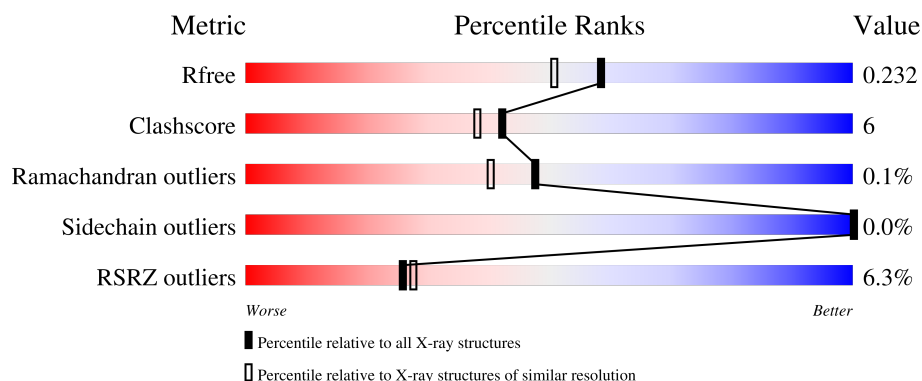
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



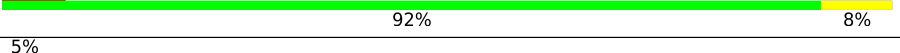
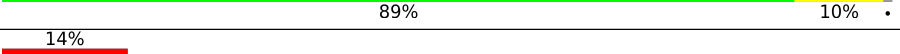
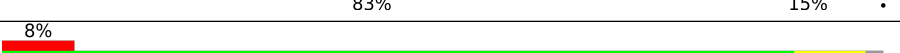
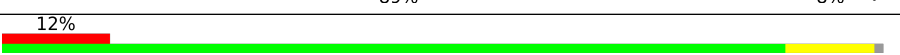
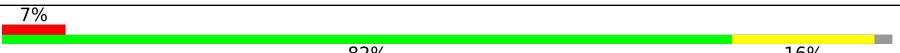
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	259	7% 91% 8%
1	B	259	7% 83% 15%
1	C	259	4% 89% 10%
1	D	259	5% 85% 15%
1	E	259	4% 88% 10%

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Mol	Chain	Length	Quality of chain
1	F	259	
1	G	259	
1	H	259	
1	I	259	
1	J	259	
1	K	259	
1	L	259	
1	M	259	
1	N	259	
1	O	259	
1	P	259	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33083 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

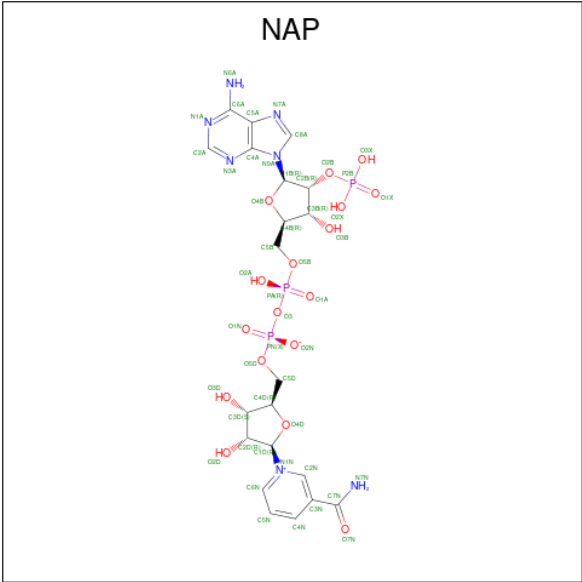
- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	B	255	Total	C	N	O	S	0	0	0
			1856	1153	327	370	6			
1	C	258	Total	C	N	O	S	0	0	0
			1875	1165	330	374	6			
1	D	259	Total	C	N	O	S	0	0	0
			1880	1168	331	375	6			
1	E	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			
1	F	254	Total	C	N	O	S	0	0	0
			1848	1147	326	369	6			
1	G	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	H	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	I	258	Total	C	N	O	S	0	0	0
			1874	1165	330	373	6			
1	J	257	Total	C	N	O	S	0	0	0
			1869	1162	329	372	6			
1	K	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			
1	L	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	M	256	Total	C	N	O	S	0	0	0
			1862	1156	328	372	6			
1	N	254	Total	C	N	O	S	0	0	0
			1848	1147	326	369	6			
1	O	253	Total	C	N	O	S	0	0	0
			1838	1141	323	368	6			
1	P	255	Total	C	N	O	S	0	0	0
			1854	1150	327	371	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0QP46
A	0	HIS	-	expression tag	UNP A0QP46
B	-1	SER	-	expression tag	UNP A0QP46
B	0	HIS	-	expression tag	UNP A0QP46
C	-1	SER	-	expression tag	UNP A0QP46
C	0	HIS	-	expression tag	UNP A0QP46
D	-1	SER	-	expression tag	UNP A0QP46
D	0	HIS	-	expression tag	UNP A0QP46
E	-1	SER	-	expression tag	UNP A0QP46
E	0	HIS	-	expression tag	UNP A0QP46
F	-1	SER	-	expression tag	UNP A0QP46
F	0	HIS	-	expression tag	UNP A0QP46
G	-1	SER	-	expression tag	UNP A0QP46
G	0	HIS	-	expression tag	UNP A0QP46
H	-1	SER	-	expression tag	UNP A0QP46
H	0	HIS	-	expression tag	UNP A0QP46
I	-1	SER	-	expression tag	UNP A0QP46
I	0	HIS	-	expression tag	UNP A0QP46
J	-1	SER	-	expression tag	UNP A0QP46
J	0	HIS	-	expression tag	UNP A0QP46
K	-1	SER	-	expression tag	UNP A0QP46
K	0	HIS	-	expression tag	UNP A0QP46
L	-1	SER	-	expression tag	UNP A0QP46
L	0	HIS	-	expression tag	UNP A0QP46
M	-1	SER	-	expression tag	UNP A0QP46
M	0	HIS	-	expression tag	UNP A0QP46
N	-1	SER	-	expression tag	UNP A0QP46
N	0	HIS	-	expression tag	UNP A0QP46
O	-1	SER	-	expression tag	UNP A0QP46
O	0	HIS	-	expression tag	UNP A0QP46
P	-1	SER	-	expression tag	UNP A0QP46
P	0	HIS	-	expression tag	UNP A0QP46

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



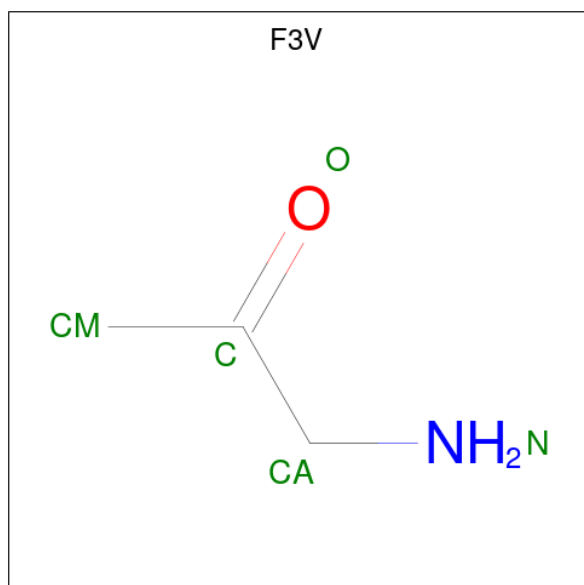
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	M	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 1-aminopropan-2-one (CCD ID: F3V) (formula: C₃H₇NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			5	3	1	1			
3	B	1	Total	C	N	O		0	0
			5	3	1	1			
3	C	1	Total	C	N	O		0	0
			5	3	1	1			
3	D	1	Total	C	N	O		0	0
			5	3	1	1			
3	E	1	Total	C	N	O		0	0
			5	3	1	1			
3	F	1	Total	C	N	O		0	0
			5	3	1	1			
3	G	1	Total	C	N	O		0	0
			5	3	1	1			
3	H	1	Total	C	N	O		0	0
			5	3	1	1			
3	I	1	Total	C	N	O		0	0
			5	3	1	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	K	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	M	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	O	1	Total	C	N	O	0	0
			5	3	1	1		
3	P	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		
4	I	1	Total	Cl	0	0
			1	1		
4	J	1	Total	Cl	0	0
			1	1		
4	K	1	Total	Cl	0	0
			1	1		
4	L	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total 1	Cl 1	0	0
4	N	1	Total 1	Cl 1	0	0
4	O	1	Total 1	Cl 1	0	0
4	P	1	Total 1	Cl 1	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0
5	H	1	Total 1	Mg 1	0	0
5	J	1	Total 1	Mg 1	0	0
5	L	1	Total 1	Mg 1	0	0
5	M	1	Total 1	Mg 1	0	0
5	O	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	223	Total 223	O 223	0	0
6	B	180	Total 180	O 180	0	0
6	C	189	Total 189	O 189	0	0
6	D	191	Total 191	O 191	0	0
6	E	202	Total 202	O 202	0	0

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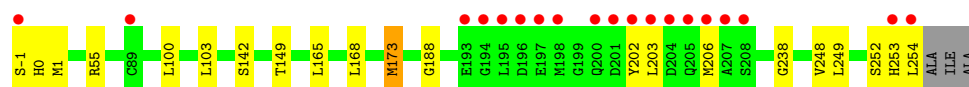
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	203	Total 203	O 203	0	0
6	G	186	Total 186	O 186	0	0
6	H	209	Total 209	O 209	0	0
6	I	106	Total 106	O 106	0	0
6	J	113	Total 113	O 113	0	0
6	K	96	Total 96	O 96	0	0
6	L	123	Total 123	O 123	0	0
6	M	111	Total 111	O 111	0	0
6	N	118	Total 118	O 118	0	0
6	O	132	Total 132	O 132	0	0
6	P	116	Total 116	O 116	0	0

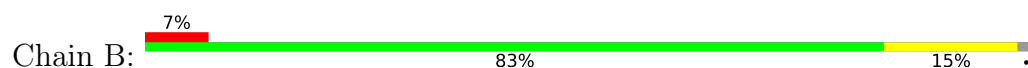
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

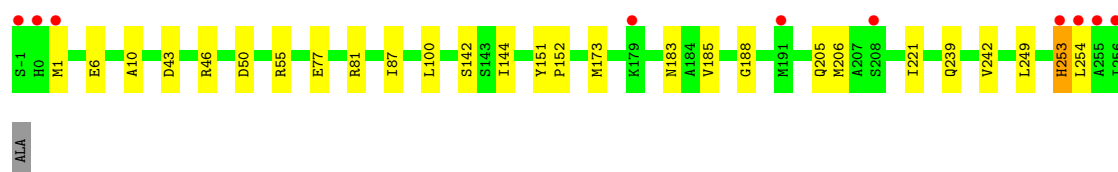
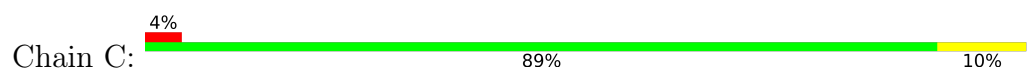
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



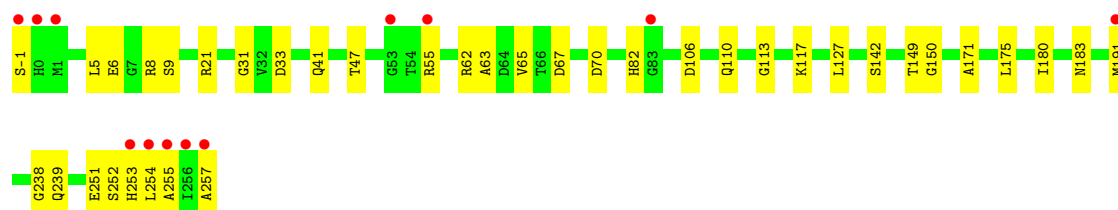
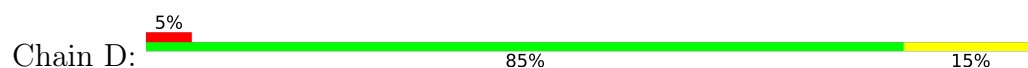
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



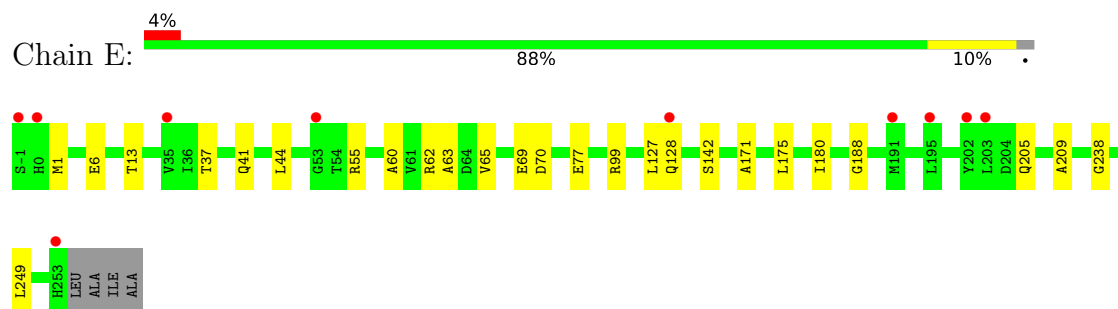
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



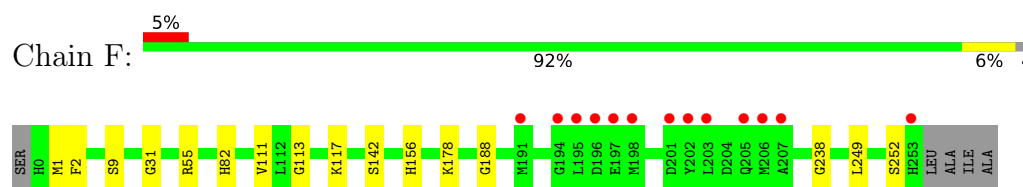
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



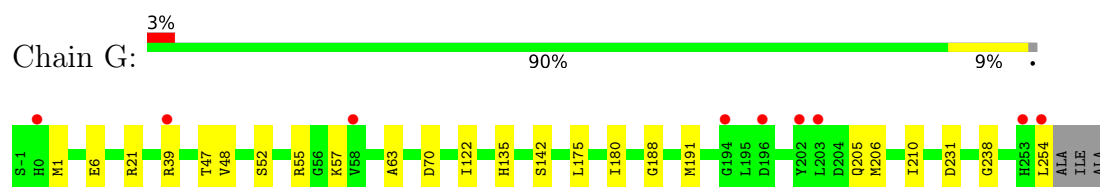
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



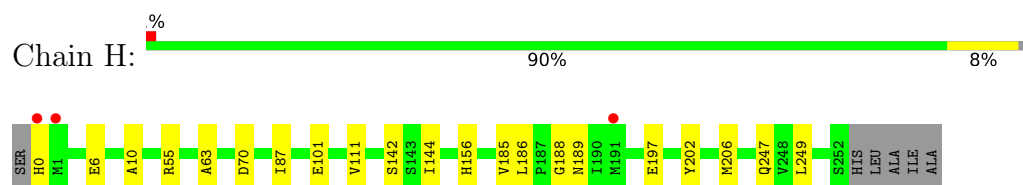
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



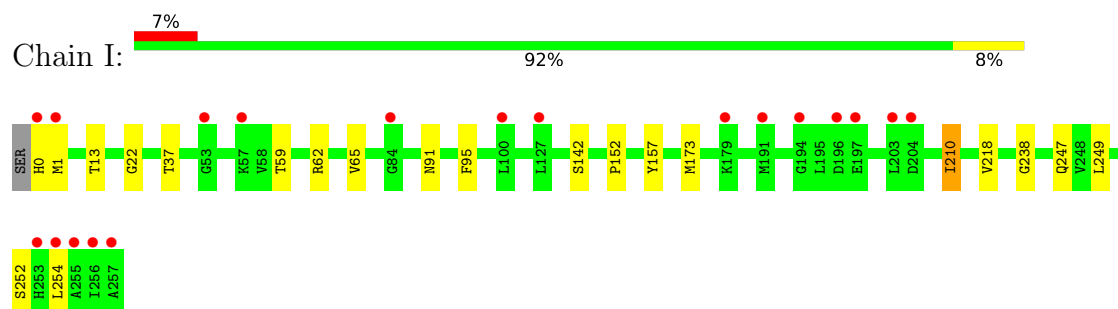
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



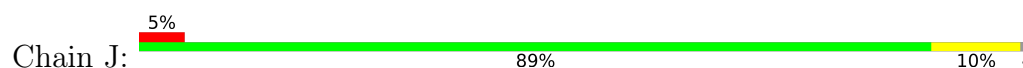
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

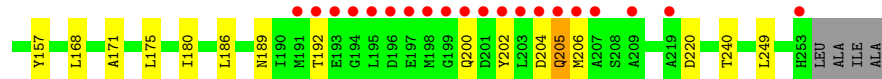
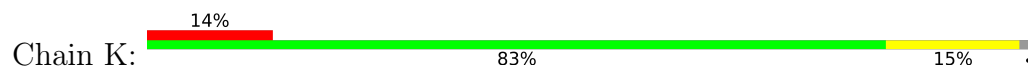


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

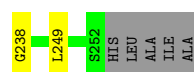
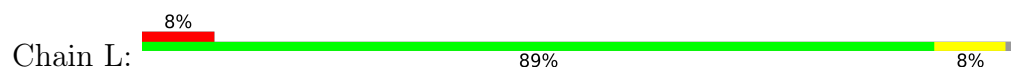




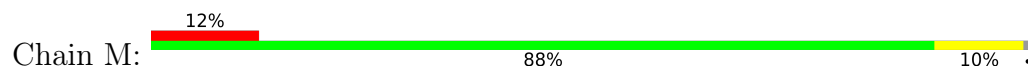
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



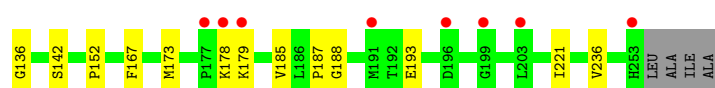
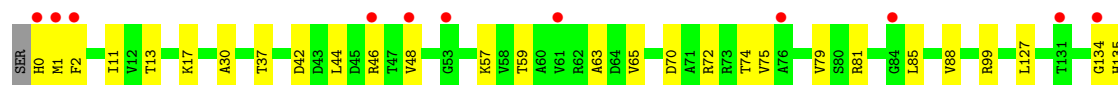
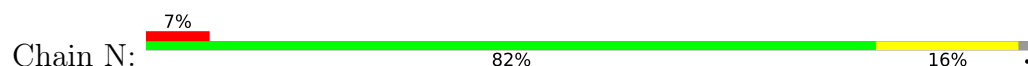
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



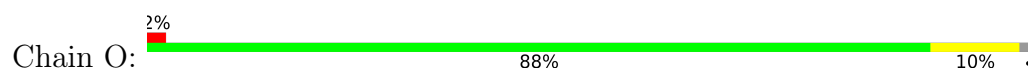
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

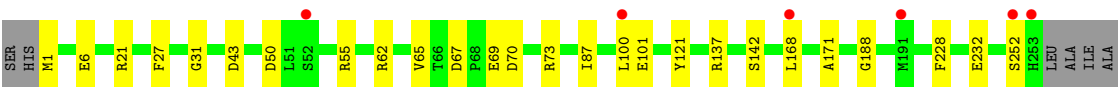


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

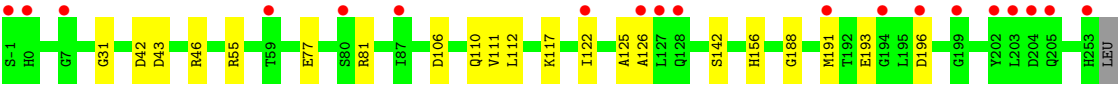
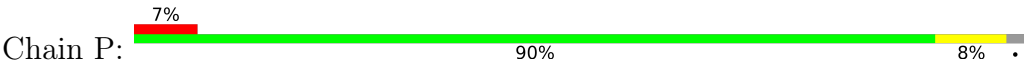


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase





● Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.77Å 129.06Å 145.79Å 90.00° 107.88° 90.00°	Depositor
Resolution (Å)	48.49 – 1.90 48.49 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.49-1.90) 99.7 (48.49-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.204 , 0.233 0.203 , 0.232	Depositor DCC
R_{free} test set	27768 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33083	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3678e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F3V, CL, MG, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/1889	0.56	1/2568 (0.0%)
1	B	0.38	0/1883	0.55	0/2560
1	C	0.39	0/1902	0.56	0/2586
1	D	0.38	0/1907	0.57	0/2593
1	E	0.38	0/1881	0.57	0/2557
1	F	0.38	0/1875	0.55	0/2549
1	G	0.34	0/1889	0.52	0/2568
1	H	0.36	0/1864	0.54	0/2534
1	I	0.30	1/1901 (0.1%)	0.46	1/2585 (0.0%)
1	J	0.26	1/1896 (0.1%)	0.42	0/2578
1	K	0.26	0/1881	0.46	0/2557
1	L	0.24	0/1864	0.44	0/2534
1	M	0.24	0/1889	0.42	0/2568
1	N	0.26	0/1875	0.46	0/2549
1	O	0.23	0/1864	0.43	0/2534
1	P	0.23	0/1881	0.43	0/2557
All	All	0.32	2/30141 (0.0%)	0.50	2/40977 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	210	ILE	CA-C	7.76	1.59	1.53
1	J	210	ILE	CA-C	-5.47	1.48	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	MET	CG-SD-CE	-5.71	88.35	100.90
1	I	210	ILE	O-C-N	5.47	125.73	121.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1862	0	1848	25	0
1	B	1856	0	1843	40	0
1	C	1875	0	1864	30	0
1	D	1880	0	1869	40	0
1	E	1854	0	1837	23	0
1	F	1848	0	1832	15	0
1	G	1862	0	1848	21	0
1	H	1838	0	1825	17	0
1	I	1874	0	1864	23	0
1	J	1869	0	1859	21	0
1	K	1854	0	1837	36	0
1	L	1838	0	1825	21	0
1	M	1862	0	1848	28	0
1	N	1848	0	1832	50	0
1	O	1838	0	1825	21	0
1	P	1854	0	1837	18	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
2	E	48	0	25	2	0
2	F	48	0	25	2	0
2	G	48	0	25	2	0
2	H	48	0	25	1	0
2	I	48	0	25	3	0
2	J	48	0	25	1	0
2	K	48	0	25	2	0
2	L	48	0	25	2	0
2	M	48	0	25	2	0
2	N	48	0	25	5	0
2	O	48	0	25	3	0
2	P	48	0	25	2	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
4	A	2	0	0	1	0
4	B	1	0	0	1	0
4	C	1	0	0	1	0
4	D	1	0	0	1	0
4	E	1	0	0	1	0
4	F	1	0	0	1	0
4	G	1	0	0	1	0
4	H	1	0	0	1	0
4	I	1	0	0	1	0
4	J	1	0	0	1	0
4	K	1	0	0	1	0
4	L	1	0	0	1	0
4	M	1	0	0	1	0
4	N	1	0	0	1	0
4	O	1	0	0	1	0
4	P	1	0	0	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
6	A	223	0	0	6	1
6	B	180	0	0	11	0
6	C	189	0	0	3	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	191	0	0	10	1
6	E	202	0	0	10	0
6	F	203	0	0	2	1
6	G	186	0	0	11	0
6	H	209	0	0	2	1
6	I	106	0	0	5	0
6	J	113	0	0	2	0
6	K	96	0	0	8	0
6	L	123	0	0	6	0
6	M	111	0	0	5	0
6	N	118	0	0	9	0
6	O	132	0	0	4	0
6	P	116	0	0	7	0
All	All	33083	0	29893	380	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (380) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:134:GLY:H	1:N:179:LYS:NZ	1.35	1.23
1:N:134:GLY:N	1:N:179:LYS:NZ	1.94	1.14
1:E:99:ARG:NH1	6:E:401:HOH:O	1.83	1.10
1:N:134:GLY:H	1:N:179:LYS:HZ3	1.08	1.01
1:B:17:LYS:NZ	6:B:401:HOH:O	1.94	1.00
1:B:55:ARG:NH2	6:B:402:HOH:O	1.99	0.95
1:K:128:GLN:NE2	6:K:403:HOH:O	1.98	0.94
1:M:1:MET:O	6:M:401:HOH:O	1.88	0.92
1:G:39:ARG:O	6:G:401:HOH:O	1.89	0.90
1:M:55:ARG:HH12	1:N:0:HIS:N	1.70	0.90
1:E:55:ARG:NH2	6:E:407:HOH:O	2.03	0.90
1:E:69:GLU:OE2	6:E:402:HOH:O	1.91	0.89
1:K:128:GLN:OE1	6:K:401:HOH:O	1.91	0.89
6:G:403:HOH:O	1:H:0:HIS:N	2.05	0.89
1:N:17:LYS:NZ	6:N:405:HOH:O	2.03	0.89
1:B:0:HIS:N	6:B:403:HOH:O	2.07	0.88
1:L:103:LEU:O	6:L:401:HOH:O	1.90	0.87
1:K:108:ILE:O	1:K:112:LEU:HD12	1.74	0.87
1:K:220:ASP:OD2	6:K:402:HOH:O	1.92	0.86
1:G:52:SER:O	6:G:402:HOH:O	1.93	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:HE1	1:D:150:GLY:HA3	1.56	0.85
1:N:134:GLY:N	1:N:179:LYS:HZ3	1.66	0.85
1:A:103:LEU:O	6:A:401:HOH:O	1.95	0.84
1:D:41:GLN:H	1:D:62:ARG:HH21	1.23	0.83
1:N:134:GLY:N	1:N:179:LYS:HZ2	1.72	0.83
1:G:57:LYS:NZ	6:G:406:HOH:O	2.12	0.81
1:E:1:MET:O	6:E:403:HOH:O	1.99	0.81
1:N:1:MET:O	6:N:401:HOH:O	1.98	0.80
1:G:48:VAL:O	6:G:404:HOH:O	2.00	0.79
1:N:135:HIS:N	1:N:179:LYS:HD3	1.96	0.79
1:N:30:ALA:O	6:N:402:HOH:O	2.00	0.79
1:D:191:MET:SD	6:D:456:HOH:O	2.41	0.78
1:D:33:ASP:OD1	6:D:402:HOH:O	2.02	0.78
1:J:94:ILE:H	1:J:115:ASN:HD21	1.28	0.77
1:E:65:VAL:O	6:E:405:HOH:O	2.03	0.76
1:E:6:GLU:OE2	6:E:404:HOH:O	2.03	0.76
2:I:301:NAP:O1X	6:I:401:HOH:O	2.03	0.76
1:E:77:GLU:OE2	6:E:406:HOH:O	2.03	0.76
1:P:122:ILE:O	6:P:401:HOH:O	2.03	0.76
1:N:48:VAL:O	6:N:403:HOH:O	2.02	0.76
1:J:52:SER:O	6:J:401:HOH:O	2.03	0.76
1:A:1:MET:O	6:A:402:HOH:O	2.01	0.76
1:P:43:ASP:HA	1:P:46:ARG:HD3	1.68	0.75
1:N:72:ARG:O	6:N:404:HOH:O	2.02	0.75
1:H:189:ASN:HD22	1:H:247:GLN:HE22	1.34	0.75
1:O:6:GLU:OE2	1:O:55:ARG:HD3	1.87	0.74
1:A:254:LEU:HD22	1:C:205:GLN:HE21	1.49	0.74
1:D:55:ARG:NH1	6:D:403:HOH:O	2.06	0.73
1:M:55:ARG:HH12	1:N:0:HIS:H3	1.34	0.73
1:L:1:MET:O	6:L:402:HOH:O	2.05	0.73
1:I:0:HIS:N	1:L:55:ARG:HH12	1.86	0.73
4:A:303:CL:CL	4:D:303:CL:CL	2.81	0.73
1:B:62:ARG:NH1	6:B:409:HOH:O	2.21	0.73
1:J:1:MET:O	6:J:402:HOH:O	2.07	0.72
1:M:59:THR:OG1	6:M:402:HOH:O	2.06	0.72
1:D:41:GLN:NE2	6:D:401:HOH:O	1.96	0.72
1:O:101:GLU:OE1	6:O:402:HOH:O	2.09	0.71
1:C:173:MET:HE1	1:D:255:ALA:HB1	1.73	0.71
1:N:59:THR:OG1	6:N:407:HOH:O	2.07	0.70
1:N:193:GLU:OE1	6:N:408:HOH:O	2.10	0.70
1:A:173:MET:HE1	1:D:150:GLY:CA	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:GLN:HG2	6:E:437:HOH:O	1.90	0.70
1:O:62:ARG:O	1:O:73:ARG:NH2	2.25	0.70
1:C:1:MET:O	6:C:402:HOH:O	2.09	0.70
1:G:1:MET:O	6:G:405:HOH:O	2.09	0.70
1:N:134:GLY:CA	1:N:179:LYS:HZ3	2.04	0.70
1:A:100:LEU:HD22	1:D:127:LEU:HD11	1.73	0.70
1:B:37:THR:O	6:B:404:HOH:O	2.09	0.70
1:D:110:GLN:OE1	6:D:404:HOH:O	2.10	0.70
1:O:121:TYR:OH	6:O:401:HOH:O	2.08	0.70
1:O:1:MET:O	6:O:403:HOH:O	2.11	0.69
1:L:17:LYS:NZ	6:L:403:HOH:O	2.26	0.69
1:I:59:THR:OG1	6:I:402:HOH:O	2.11	0.68
1:I:173:MET:HE1	1:J:150:GLY:C	2.19	0.67
1:I:62:ARG:NE	6:I:405:HOH:O	2.25	0.67
1:P:196:ASP:OD2	6:P:402:HOH:O	2.13	0.67
1:A:254:LEU:CD2	1:C:205:GLN:HE21	2.08	0.66
1:N:136:GLY:H	1:N:179:LYS:CD	2.09	0.66
1:E:127:LEU:HD21	1:E:175:LEU:HD22	1.76	0.66
1:M:196:ASP:OD1	6:M:403:HOH:O	2.15	0.65
1:P:125:ALA:N	6:P:401:HOH:O	2.29	0.65
1:D:67:ASP:OD1	6:D:405:HOH:O	2.14	0.65
1:O:6:GLU:HG2	1:O:31:GLY:HA3	1.79	0.65
2:B:301:NAP:H2A	6:B:440:HOH:O	1.94	0.65
1:L:21:ARG:HD3	6:L:506:HOH:O	1.96	0.64
1:B:206:MET:HE1	1:D:251:GLU:HG2	1.80	0.64
1:P:31:GLY:HA2	1:P:55:ARG:HG2	1.80	0.64
1:B:69:GLU:OE1	6:B:405:HOH:O	2.14	0.64
1:D:82:HIS:HE1	6:D:438:HOH:O	1.79	0.64
1:B:142:SER:O	2:B:301:NAP:H6N	1.98	0.63
1:I:152:PRO:HD3	1:J:173:MET:HE2	1.80	0.63
4:F:303:CL:CL	4:G:303:CL:CL	2.90	0.63
1:I:0:HIS:H1	1:L:55:ARG:HH12	1.45	0.63
1:N:136:GLY:H	1:N:179:LYS:HD3	1.63	0.63
1:H:101:GLU:OE1	6:H:402:HOH:O	2.16	0.63
1:N:134:GLY:CA	1:N:179:LYS:NZ	2.60	0.63
1:C:50:ASP:OD2	6:C:403:HOH:O	2.16	0.63
1:F:252:SER:HB3	1:H:206:MET:CE	2.29	0.62
1:B:69:GLU:HG2	1:B:72:ARG:HH21	1.64	0.61
4:E:303:CL:CL	4:H:303:CL:CL	2.92	0.61
1:C:55:ARG:CZ	1:D:-1:SER:HB2	2.31	0.61
1:G:142:SER:O	2:G:301:NAP:H6N	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:O	6:B:406:HOH:O	2.16	0.60
1:J:6:GLU:HG3	1:J:31:GLY:HA3	1.82	0.60
1:H:111:VAL:HG21	1:H:156:HIS:CD2	2.36	0.60
1:B:183:ASN:HD22	1:B:239:GLN:H	1.47	0.60
1:A:142:SER:O	2:A:301:NAP:H6N	2.01	0.60
1:G:191:MET:SD	6:G:535:HOH:O	2.57	0.60
1:N:42:ASP:O	1:N:46:ARG:HG2	2.01	0.60
1:K:77:GLU:O	1:K:81:ARG:HG3	2.01	0.60
1:K:65:VAL:HA	6:K:460:HOH:O	2.01	0.60
1:F:252:SER:HB3	1:H:206:MET:HE1	1.85	0.59
1:K:125:ALA:O	6:K:401:HOH:O	2.17	0.59
1:K:128:GLN:CD	6:K:401:HOH:O	2.41	0.59
1:P:142:SER:O	2:P:301:NAP:H6N	2.01	0.59
1:B:55:ARG:HG3	6:B:412:HOH:O	2.01	0.59
1:B:209:ALA:HB1	1:B:253:HIS:CD2	2.38	0.59
1:I:142:SER:O	2:I:301:NAP:H6N	2.03	0.59
1:E:41:GLN:HE21	1:E:62:ARG:NH1	2.01	0.58
1:B:188:GLY:O	2:B:301:NAP:H4N	2.02	0.58
1:I:254:LEU:HD13	1:K:205:GLN:HA	1.85	0.58
4:N:303:CL:CL	4:O:303:CL:CL	2.95	0.58
1:L:31:GLY:HA2	1:L:55:ARG:HG2	1.86	0.58
1:D:142:SER:O	2:D:301:NAP:H6N	2.03	0.57
4:B:303:CL:CL	4:C:303:CL:CL	2.97	0.57
1:M:112:LEU:HD21	1:P:112:LEU:HD12	1.86	0.57
1:N:63:ALA:HB1	1:N:70:ASP:HB3	1.86	0.57
1:G:135:HIS:O	6:G:407:HOH:O	2.17	0.57
1:E:142:SER:O	2:E:301:NAP:H6N	2.05	0.57
1:D:67:ASP:OD2	6:D:406:HOH:O	2.17	0.56
1:D:171:ALA:O	1:D:175:LEU:HG	2.06	0.56
1:K:57:LYS:HG2	1:N:81:ARG:O	2.05	0.56
1:N:135:HIS:CA	1:N:179:LYS:HD3	2.35	0.56
1:O:43:ASP:O	6:O:404:HOH:O	2.18	0.56
1:E:205:GLN:NE2	6:E:412:HOH:O	2.33	0.56
1:H:6:GLU:OE2	1:H:55:ARG:HD2	2.04	0.56
1:F:142:SER:O	2:F:301:NAP:H6N	2.05	0.56
1:M:155:SER:HB3	6:M:413:HOH:O	2.03	0.56
1:N:44:LEU:O	1:N:48:VAL:HG12	2.06	0.56
1:P:77:GLU:O	1:P:81:ARG:HG3	2.05	0.56
1:D:6:GLU:O	6:D:407:HOH:O	2.18	0.56
1:B:152:PRO:HD2	1:D:255:ALA:HA	1.88	0.55
1:N:134:GLY:C	1:N:179:LYS:HD3	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:SER:O	2:L:301:NAP:H6N	2.07	0.55
1:C:183:ASN:HD22	1:C:239:GLN:H	1.55	0.55
1:M:206:MET:O	1:M:210:ILE:HG13	2.06	0.55
1:C:77:GLU:O	1:C:81:ARG:HG3	2.07	0.55
1:G:188:GLY:O	2:G:301:NAP:H4N	2.06	0.54
4:K:303:CL:CL	4:L:303:CL:CL	2.99	0.54
1:F:9:SER:OG	1:F:82:HIS:HD2	1.90	0.54
1:N:127:LEU:HD21	1:N:178:LYS:HD3	1.90	0.54
1:D:41:GLN:HB2	1:D:62:ARG:HE	1.73	0.54
1:G:254:LEU:H	1:G:254:LEU:HD23	1.72	0.54
1:E:55:ARG:CZ	6:E:407:HOH:O	2.48	0.53
1:A:252:SER:HB3	1:C:206:MET:HE1	1.90	0.53
1:L:0:HIS:N	6:L:409:HOH:O	2.40	0.53
1:B:205:GLN:NE2	1:D:252:SER:OG	2.42	0.53
1:K:142:SER:O	2:K:301:NAP:H6N	2.09	0.53
1:K:189:ASN:CG	1:K:206:MET:HG3	2.33	0.53
1:E:238:GLY:HA3	1:F:249:LEU:HD11	1.90	0.53
1:A:254:LEU:HD22	1:C:205:GLN:NE2	2.23	0.53
1:K:128:GLN:NE2	6:K:401:HOH:O	2.42	0.53
1:P:126:ALA:N	6:P:401:HOH:O	2.07	0.52
1:H:142:SER:O	2:H:301:NAP:H6N	2.10	0.52
1:N:178:LYS:O	1:N:179:LYS:HB3	2.07	0.52
1:K:175:LEU:HB3	1:K:180:ILE:HB	1.91	0.52
1:I:254:LEU:HD22	1:K:205:GLN:HB2	1.91	0.52
1:M:36:ILE:HD12	1:M:44:LEU:HD23	1.92	0.52
1:D:183:ASN:HD22	1:D:239:GLN:H	1.57	0.51
1:P:122:ILE:C	6:P:401:HOH:O	2.52	0.51
1:C:43:ASP:OD2	1:C:46:ARG:NH2	2.42	0.51
1:I:65:VAL:O	6:I:403:HOH:O	2.19	0.51
1:K:63:ALA:HB1	1:K:70:ASP:HB3	1.92	0.51
1:E:188:GLY:O	2:E:301:NAP:H4N	2.10	0.51
1:B:167:PHE:HE1	1:C:100:LEU:HD13	1.76	0.51
1:A:188:GLY:O	2:A:301:NAP:H4N	2.10	0.51
1:B:80:SER:OG	6:B:407:HOH:O	2.19	0.51
1:J:142:SER:O	2:J:301:NAP:H6N	2.11	0.51
1:H:206:MET:HA	1:H:206:MET:HE2	1.93	0.51
1:P:106:ASP:O	1:P:110:GLN:HG2	2.11	0.51
1:B:17:LYS:NZ	1:B:43:ASP:OD2	2.36	0.50
1:D:5:LEU:O	1:D:8:ARG:HG3	2.11	0.50
1:P:188:GLY:O	2:P:301:NAP:H4N	2.12	0.50
1:A:202:TYR:HD1	1:A:203:LEU:HD12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:TYR:HA	1:K:205:GLN:HE21	1.77	0.50
1:F:1:MET:O	6:F:401:HOH:O	2.18	0.50
1:J:0:HIS:N	1:K:55:ARG:HH21	2.10	0.50
1:G:63:ALA:HB1	1:G:70:ASP:HB3	1.93	0.50
1:I:0:HIS:N	1:L:55:ARG:NH1	2.59	0.50
1:A:-1:SER:HB3	1:B:55:ARG:HE	1.77	0.50
1:A:248:VAL:O	6:A:403:HOH:O	2.19	0.50
1:K:200:GLN:HG3	1:K:204:ASP:OD2	2.12	0.50
1:N:134:GLY:H	1:N:179:LYS:HZ1	1.45	0.49
1:M:189:ASN:HD22	1:M:195:LEU:HD21	1.77	0.49
1:A:249:LEU:HD11	1:B:238:GLY:HA3	1.94	0.49
1:C:142:SER:O	2:C:301:NAP:H6N	2.13	0.49
1:G:6:GLU:OE1	1:G:55:ARG:NE	2.46	0.49
1:M:128:GLN:OE1	1:M:129:ALA:N	2.41	0.49
1:E:1:MET:HE3	1:F:2:PHE:HB2	1.94	0.49
4:M:303:CL:CL	4:P:303:CL:CL	3.04	0.49
1:B:193:GLU:OE1	6:B:408:HOH:O	2.20	0.49
1:D:149:THR:HG22	6:D:442:HOH:O	2.12	0.49
1:O:142:SER:O	2:O:301:NAP:H6N	2.13	0.49
1:H:144:ILE:HG12	1:H:188:GLY:HA2	1.93	0.48
1:O:137:ARG:HD2	1:O:228:PHE:O	2.12	0.48
1:M:250:PRO:HG3	1:N:173:MET:HE3	1.95	0.48
1:J:21:ARG:HH11	1:J:47:THR:HG23	1.78	0.48
1:O:27:PHE:HE1	1:O:87:ILE:HD13	1.79	0.48
1:M:183:ASN:HD22	1:M:239:GLN:H	1.61	0.48
1:A:238:GLY:HA3	1:B:249:LEU:HD11	1.96	0.48
1:D:252:SER:OG	1:D:253:HIS:N	2.47	0.48
1:H:63:ALA:HB1	1:H:70:ASP:HB3	1.96	0.48
1:O:232:GLU:N	1:O:232:GLU:OE2	2.47	0.48
1:D:254:LEU:HG	1:D:257:ALA:C	2.39	0.47
1:M:1:MET:HE1	1:N:2:PHE:HB2	1.96	0.47
1:G:238:GLY:HA3	1:H:249:LEU:HD11	1.96	0.47
1:N:65:VAL:HA	6:N:413:HOH:O	2.14	0.47
1:M:142:SER:O	2:M:301:NAP:H6N	2.14	0.47
1:O:27:PHE:CE1	1:O:87:ILE:HD13	2.49	0.47
1:B:205:GLN:NE2	1:D:254:LEU:H	2.12	0.47
1:K:168:LEU:HA	1:K:171:ALA:HB3	1.95	0.47
1:D:21:ARG:HD2	1:D:47:THR:HG23	1.95	0.47
1:D:106:ASP:O	1:D:110:GLN:HG2	2.15	0.47
1:G:206:MET:O	1:G:210:ILE:HG13	2.15	0.47
1:N:142:SER:O	2:N:301:NAP:H6N	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:GLN:HB2	1:D:62:ARG:NE	2.30	0.47
1:J:209:ALA:HA	1:J:256:ILE:HD13	1.97	0.47
1:E:13:THR:HA	1:E:37:THR:OG1	2.13	0.47
1:A:149:THR:HA	6:A:468:HOH:O	2.15	0.46
1:C:249:LEU:HD11	1:D:238:GLY:HA3	1.98	0.46
1:J:238:GLY:HA3	1:K:249:LEU:HD11	1.96	0.46
1:B:63:ALA:HB1	1:B:70:ASP:HB3	1.97	0.46
1:C:206:MET:HA	1:C:206:MET:HE2	1.97	0.46
1:I:1:MET:CE	1:L:2:PHE:HB2	2.46	0.46
1:F:178:LYS:HD3	6:F:521:HOH:O	2.15	0.46
1:A:173:MET:HE2	1:B:249:LEU:HB3	1.98	0.46
1:L:59:THR:HB	1:L:81:ARG:NH1	2.31	0.46
1:F:252:SER:HB3	1:H:206:MET:HE2	1.97	0.46
1:M:59:THR:HB	1:M:81:ARG:NH1	2.30	0.46
1:C:55:ARG:NE	1:D:-1:SER:HB2	2.31	0.46
1:J:115:ASN:N	1:J:115:ASN:HD22	2.12	0.46
1:I:210:ILE:HG12	1:I:247:GLN:HB2	1.98	0.46
1:B:21:ARG:NH1	1:B:46:ARG:NH1	2.63	0.45
1:E:171:ALA:O	1:E:175:LEU:HG	2.16	0.45
1:O:67:ASP:HB3	1:O:70:ASP:HB2	1.97	0.45
1:C:253:HIS:H	1:C:253:HIS:CD2	2.35	0.45
1:D:65:VAL:HG22	2:D:301:NAP:N1A	2.31	0.45
1:G:175:LEU:HB3	1:G:180:ILE:HB	1.98	0.45
1:I:173:MET:HE1	1:J:150:GLY:CA	2.46	0.45
1:A:253:HIS:HD2	6:A:564:HOH:O	1.98	0.45
1:B:183:ASN:ND2	1:B:239:GLN:H	2.14	0.45
1:N:13:THR:HA	1:N:37:THR:OG1	2.17	0.45
1:B:173:MET:CE	1:C:152:PRO:HD3	2.47	0.45
1:K:202:TYR:C	1:K:205:GLN:HB3	2.41	0.45
1:L:200:GLN:NE2	1:L:204:ASP:OD1	2.48	0.45
1:M:188:GLY:O	2:M:301:NAP:H4N	2.16	0.45
2:N:301:NAP:H2A	6:N:437:HOH:O	2.16	0.45
1:K:95:PHE:HB3	1:K:157:TYR:CE1	2.52	0.45
1:M:25:GLU:OE1	6:M:404:HOH:O	2.20	0.45
1:B:173:MET:HE1	1:C:151:TYR:HA	1.99	0.45
1:P:191:MET:HE3	1:P:191:MET:HA	1.97	0.45
1:D:31:GLY:HA2	1:D:55:ARG:HD2	1.97	0.45
1:I:91:ASN:O	2:I:301:NAP:H4D	2.17	0.45
1:M:210:ILE:HG12	1:M:247:GLN:HB2	1.98	0.45
1:A:165:LEU:HA	1:A:168:LEU:HG	1.98	0.44
1:E:175:LEU:HB3	1:E:180:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LEU:HB3	1:D:180:ILE:HB	1.99	0.44
4:I:303:CL:CL	4:J:303:CL:CL	3.09	0.44
1:N:179:LYS:HB3	1:N:179:LYS:HE2	1.69	0.44
1:K:122:ILE:HD12	1:K:122:ILE:HA	1.86	0.44
1:N:187:PRO:HB2	2:N:301:NAP:C5N	2.48	0.44
1:O:168:LEU:HA	1:O:171:ALA:HB3	1.99	0.44
1:G:231:ASP:OD2	6:G:408:HOH:O	2.21	0.44
1:L:202:TYR:CE2	1:L:206:MET:HE2	2.52	0.44
1:M:128:GLN:CD	1:M:129:ALA:H	2.25	0.44
1:I:249:LEU:HD11	1:L:238:GLY:HA3	1.98	0.44
1:E:44:LEU:HD22	1:E:60:ALA:HB1	1.99	0.44
1:G:21:ARG:HD2	1:G:47:THR:HG23	1.99	0.44
1:A:202:TYR:CE2	1:A:206:MET:HE2	2.53	0.44
1:G:55:ARG:NH1	6:G:403:HOH:O	1.95	0.44
1:M:44:LEU:HD22	1:M:60:ALA:HB1	2.00	0.44
1:N:65:VAL:HG22	2:N:301:NAP:N1A	2.33	0.44
1:N:188:GLY:O	2:N:301:NAP:H4N	2.17	0.44
1:A:0:HIS:NE2	6:A:408:HOH:O	2.36	0.44
1:M:247:GLN:O	1:M:250:PRO:HD2	2.17	0.44
1:A:55:ARG:NH1	1:B:0:HIS:N	2.66	0.43
1:B:173:MET:HE1	1:C:152:PRO:HD3	2.00	0.43
1:D:63:ALA:HB1	1:D:70:ASP:HB3	2.00	0.43
1:H:10:ALA:HA	1:H:87:ILE:O	2.18	0.43
1:I:173:MET:HE3	1:I:173:MET:HB2	1.84	0.43
1:J:13:THR:HA	1:J:37:THR:OG1	2.18	0.43
1:K:99:ARG:HA	1:K:99:ARG:HD2	1.75	0.43
1:K:128:GLN:NE2	1:K:129:ALA:H	2.16	0.43
1:F:31:GLY:HA2	1:F:55:ARG:HG2	2.00	0.43
1:G:205:GLN:NE2	6:G:423:HOH:O	2.51	0.43
1:K:108:ILE:HG23	1:K:112:LEU:CD1	2.48	0.43
1:L:77:GLU:O	1:L:81:ARG:HG3	2.18	0.43
1:N:99:ARG:NH1	1:N:152:PRO:HB3	2.32	0.43
1:E:63:ALA:HB1	1:E:70:ASP:HB3	1.99	0.43
1:J:5:LEU:O	1:J:8:ARG:HG3	2.19	0.43
1:K:19:ILE:HG13	1:K:192:THR:HG21	2.00	0.43
1:N:99:ARG:HH12	1:N:152:PRO:CB	2.32	0.43
1:J:94:ILE:H	1:J:115:ASN:ND2	2.07	0.43
1:M:243:VAL:HG13	1:N:236:VAL:HG22	2.00	0.43
1:P:193:GLU:O	1:P:196:ASP:HB2	2.18	0.43
1:I:95:PHE:HB3	1:I:157:TYR:CE1	2.54	0.43
1:B:200:GLN:HA	1:B:203:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:GLY:HA2	1:F:117:LYS:HG3	2.00	0.43
1:P:111:VAL:HG21	1:P:156:HIS:CD2	2.53	0.43
1:H:197:GLU:HG3	6:H:602:HOH:O	2.19	0.43
1:J:21:ARG:NH1	1:J:47:THR:HG23	2.34	0.43
1:B:165:LEU:HA	1:B:168:LEU:HG	2.01	0.43
1:L:128:GLN:HG2	6:L:450:HOH:O	2.18	0.43
1:M:109:GLU:OE1	1:P:117:LYS:NZ	2.48	0.43
1:B:39:ARG:HA	1:B:62:ARG:HH11	1.84	0.43
1:I:13:THR:HA	1:I:37:THR:OG1	2.19	0.42
1:K:126:ALA:O	1:K:130:LEU:HG	2.19	0.42
1:O:21:ARG:HH22	1:O:50:ASP:HB3	1.84	0.42
1:C:6:GLU:HG3	6:C:428:HOH:O	2.18	0.42
1:J:127:LEU:HD12	1:J:127:LEU:HA	1.89	0.42
1:N:179:LYS:C	1:N:179:LYS:HD2	2.44	0.42
1:A:252:SER:HB3	1:C:206:MET:CE	2.49	0.42
1:D:9:SER:OG	1:D:82:HIS:HD2	2.02	0.42
1:E:249:LEU:HD11	1:F:238:GLY:HA3	2.00	0.42
1:M:128:GLN:CD	1:M:129:ALA:N	2.77	0.42
1:C:183:ASN:ND2	1:C:239:GLN:H	2.18	0.42
1:N:136:GLY:N	1:N:179:LYS:HD3	2.31	0.42
1:O:188:GLY:O	2:O:301:NAP:H4N	2.18	0.42
1:P:196:ASP:CG	6:P:402:HOH:O	2.58	0.42
1:B:10:ALA:HA	1:B:87:ILE:O	2.19	0.42
1:B:168:LEU:HA	1:B:171:ALA:HB3	2.01	0.42
1:D:55:ARG:C	1:D:55:ARG:CD	2.93	0.42
1:M:99:ARG:HE	1:M:99:ARG:HB3	1.64	0.42
1:F:188:GLY:O	2:F:301:NAP:H4N	2.20	0.42
1:H:185:VAL:C	1:H:186:LEU:HD12	2.44	0.42
1:N:75:VAL:O	1:N:79:VAL:HG23	2.19	0.42
1:A:252:SER:CB	1:C:206:MET:HE1	2.49	0.42
1:E:209:ALA:HB2	1:G:254:LEU:HD21	2.01	0.42
1:B:206:MET:O	1:B:210:ILE:HG13	2.20	0.42
1:F:111:VAL:HG21	1:F:156:HIS:CD2	2.55	0.42
1:G:122:ILE:HD12	1:G:122:ILE:HA	1.92	0.42
1:J:253:HIS:O	1:J:256:ILE:HD12	2.19	0.42
1:K:65:VAL:HG22	2:K:301:NAP:N1A	2.36	0.41
1:M:206:MET:SD	1:O:252:SER:HB3	2.60	0.41
1:I:22:GLY:HA3	1:I:218:VAL:HB	2.03	0.41
1:K:186:LEU:HD13	1:K:240:THR:HB	2.02	0.41
1:O:65:VAL:HG22	2:O:301:NAP:N1A	2.35	0.41
1:C:10:ALA:HA	1:C:87:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:VAL:HA	6:I:468:HOH:O	2.19	0.41
1:C:185:VAL:HG11	1:C:221:ILE:HG23	2.03	0.41
1:J:27:PHE:CE1	1:J:87:ILE:HD13	2.56	0.41
1:O:6:GLU:CD	1:O:55:ARG:HD3	2.43	0.41
1:P:42:ASP:CG	6:P:410:HOH:O	2.64	0.41
1:F:9:SER:OG	1:F:82:HIS:CD2	2.72	0.41
1:H:202:TYR:CE1	1:H:206:MET:HG3	2.55	0.41
1:N:57:LYS:HB2	1:N:57:LYS:HE3	1.92	0.41
1:B:205:GLN:O	1:B:205:GLN:HG2	2.21	0.41
1:C:55:ARG:HE	1:C:55:ARG:HB2	1.61	0.41
1:I:238:GLY:HA3	1:L:249:LEU:HD11	2.01	0.41
1:N:99:ARG:HH12	1:N:152:PRO:HB3	1.85	0.41
1:O:67:ASP:OD2	1:O:69:GLU:HG2	2.21	0.41
1:D:113:GLY:HA2	1:D:117:LYS:HB2	2.02	0.41
1:J:63:ALA:HB1	1:J:70:ASP:HB3	2.03	0.41
1:B:111:VAL:HG21	1:B:156:HIS:CD2	2.56	0.40
1:M:230:THR:HG22	1:N:1:MET:HE1	2.03	0.40
1:N:85:LEU:HD11	1:N:88:VAL:HG23	2.02	0.40
1:C:253:HIS:CG	1:C:254:LEU:H	2.39	0.40
1:N:11:ILE:HD13	1:N:74:THR:HG22	2.03	0.40
1:N:167:PHE:HE2	1:O:100:LEU:HD13	1.85	0.40
1:C:242:VAL:HB	1:D:239:GLN:CD	2.47	0.40
1:I:252:SER:HB3	1:K:206:MET:SD	2.61	0.40
1:K:10:ALA:HA	1:K:87:ILE:O	2.21	0.40
1:K:44:LEU:HD22	1:K:60:ALA:HB1	2.02	0.40
1:K:73:ARG:O	1:K:77:GLU:HG2	2.21	0.40
1:L:14:GLY:HA2	2:L:301:NAP:H1B	2.03	0.40
1:L:122:ILE:HD12	1:L:122:ILE:HA	1.90	0.40
1:N:185:VAL:HG11	1:N:221:ILE:HG23	2.03	0.40
1:K:200:GLN:N	6:K:405:HOH:O	2.29	0.40
1:C:144:ILE:HG12	1:C:188:GLY:HA2	2.04	0.40
1:L:95:PHE:HB3	1:L:157:TYR:CE1	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:577:HOH:O	6:C:558:HOH:O[2_948]	1.96	0.24
6:C:582:HOH:O	6:D:534:HOH:O[2_958]	2.14	0.06
6:F:470:HOH:O	6:H:566:HOH:O[2_859]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/259 (98%)	244 (96%)	10 (4%)	0	100	100
1	B	253/259 (98%)	246 (97%)	7 (3%)	0	100	100
1	C	256/259 (99%)	244 (95%)	11 (4%)	1 (0%)	30	22
1	D	257/259 (99%)	246 (96%)	11 (4%)	0	100	100
1	E	253/259 (98%)	246 (97%)	7 (3%)	0	100	100
1	F	252/259 (97%)	241 (96%)	11 (4%)	0	100	100
1	G	254/259 (98%)	245 (96%)	9 (4%)	0	100	100
1	H	251/259 (97%)	240 (96%)	11 (4%)	0	100	100
1	I	256/259 (99%)	245 (96%)	11 (4%)	0	100	100
1	J	255/259 (98%)	243 (95%)	11 (4%)	1 (0%)	30	22
1	K	253/259 (98%)	243 (96%)	9 (4%)	1 (0%)	30	22
1	L	251/259 (97%)	243 (97%)	8 (3%)	0	100	100
1	M	254/259 (98%)	242 (95%)	12 (5%)	0	100	100
1	N	252/259 (97%)	240 (95%)	12 (5%)	0	100	100
1	O	251/259 (97%)	242 (96%)	9 (4%)	0	100	100
1	P	253/259 (98%)	241 (95%)	12 (5%)	0	100	100
All	All	4055/4144 (98%)	3891 (96%)	161 (4%)	3 (0%)	48	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	253	HIS
1	K	205	GLN
1	C	253	HIS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/194 (100%)	193 (100%)	0	100	100
1	B	192/194 (99%)	192 (100%)	0	100	100
1	C	194/194 (100%)	194 (100%)	0	100	100
1	D	194/194 (100%)	194 (100%)	0	100	100
1	E	192/194 (99%)	192 (100%)	0	100	100
1	F	191/194 (98%)	191 (100%)	0	100	100
1	G	193/194 (100%)	193 (100%)	0	100	100
1	H	190/194 (98%)	190 (100%)	0	100	100
1	I	193/194 (100%)	193 (100%)	0	100	100
1	J	193/194 (100%)	193 (100%)	0	100	100
1	K	192/194 (99%)	192 (100%)	0	100	100
1	L	190/194 (98%)	189 (100%)	1 (0%)	81	84
1	M	193/194 (100%)	193 (100%)	0	100	100
1	N	191/194 (98%)	191 (100%)	0	100	100
1	O	190/194 (98%)	190 (100%)	0	100	100
1	P	192/194 (99%)	192 (100%)	0	100	100
All	All	3073/3104 (99%)	3072 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	128	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	91	ASN

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Mol	Chain	Res	Type
1	B	183	ASN
1	B	205	GLN
1	C	183	ASN
1	C	205	GLN
1	C	223	ASN
1	D	82	HIS
1	D	183	ASN
1	D	189	ASN
1	D	223	ASN
1	D	239	GLN
1	E	0	HIS
1	E	41	GLN
1	E	239	GLN
1	F	82	HIS
1	F	124	GLN
1	F	253	HIS
1	G	0	HIS
1	G	41	GLN
1	G	135	HIS
1	G	189	ASN
1	G	223	ASN
1	H	91	ASN
1	H	124	GLN
1	H	247	GLN
1	I	189	ASN
1	J	115	ASN
1	J	189	ASN
1	J	205	GLN
1	J	223	ASN
1	K	124	GLN
1	L	91	ASN
1	L	110	GLN
1	M	183	ASN
1	M	189	ASN
1	M	200	GLN
1	M	239	GLN
1	N	41	GLN
1	N	189	ASN
1	O	135	HIS
1	O	189	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 25 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	F3V	J	302	-	4,4,4	0.87	0	3,4,4	1.60	1 (33%)
3	F3V	A	302	-	4,4,4	0.73	0	3,4,4	2.20	1 (33%)
3	F3V	E	302	-	4,4,4	1.11	0	3,4,4	2.34	1 (33%)
2	NAP	A	301	-	50,52,52	2.84	19 (38%)	71,80,80	2.16	16 (22%)
2	NAP	J	301	5	50,52,52	2.85	20 (40%)	71,80,80	2.16	15 (21%)
2	NAP	N	301	-	50,52,52	2.91	20 (40%)	71,80,80	2.23	16 (22%)
3	F3V	O	302	-	4,4,4	0.76	0	3,4,4	1.91	1 (33%)
2	NAP	L	301	-	50,52,52	2.88	20 (40%)	71,80,80	2.22	15 (21%)
3	F3V	B	302	-	4,4,4	0.81	0	3,4,4	3.01	2 (66%)
3	F3V	P	302	-	4,4,4	0.85	0	3,4,4	2.11	1 (33%)
3	F3V	H	302	-	4,4,4	0.69	0	3,4,4	2.51	2 (66%)
2	NAP	B	301	-	50,52,52	2.93	20 (40%)	71,80,80	2.22	20 (28%)
2	NAP	E	301	-	50,52,52	2.83	21 (42%)	71,80,80	2.22	17 (23%)
3	F3V	K	302	-	4,4,4	0.90	0	3,4,4	2.22	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	F3V	C	302	-	4,4,4	0.81	0	3,4,4	1.59	1 (33%)
3	F3V	D	302	-	4,4,4	0.89	0	3,4,4	1.21	0
3	F3V	G	302	-	4,4,4	0.94	0	3,4,4	1.69	1 (33%)
3	F3V	F	302	-	4,4,4	0.89	0	3,4,4	1.77	1 (33%)
3	F3V	L	302	-	4,4,4	0.82	0	3,4,4	2.07	1 (33%)
2	NAP	D	301	-	50,52,52	2.82	18 (36%)	71,80,80	2.29	17 (23%)
2	NAP	G	301	-	50,52,52	2.85	18 (36%)	71,80,80	2.25	15 (21%)
2	NAP	F	301	-	50,52,52	2.80	20 (40%)	71,80,80	2.19	18 (25%)
2	NAP	O	301	5	50,52,52	2.86	19 (38%)	71,80,80	2.30	15 (21%)
3	F3V	N	302	-	4,4,4	1.02	0	3,4,4	1.89	1 (33%)
2	NAP	P	301	-	50,52,52	2.80	20 (40%)	71,80,80	2.24	15 (21%)
3	F3V	M	302	-	4,4,4	0.87	0	3,4,4	2.28	1 (33%)
2	NAP	K	301	-	50,52,52	2.86	20 (40%)	71,80,80	2.25	16 (22%)
2	NAP	C	301	5	50,52,52	2.58	17 (34%)	71,80,80	2.21	16 (22%)
2	NAP	M	301	-	50,52,52	2.95	19 (38%)	71,80,80	2.17	16 (22%)
2	NAP	I	301	-	50,52,52	2.87	20 (40%)	71,80,80	2.19	17 (23%)
2	NAP	H	301	5	50,52,52	2.69	18 (36%)	71,80,80	2.28	16 (22%)
3	F3V	I	302	-	4,4,4	0.83	0	3,4,4	2.80	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	F3V	J	302	-	-	0/1/2/2	-
3	F3V	A	302	-	-	0/1/2/2	-
3	F3V	E	302	-	-	0/1/2/2	-
2	NAP	A	301	-	-	6/35/67/67	0/5/5/5
2	NAP	J	301	5	-	2/35/67/67	0/5/5/5
2	NAP	N	301	-	-	3/35/67/67	0/5/5/5
3	F3V	O	302	-	-	0/1/2/2	-
2	NAP	L	301	-	-	4/35/67/67	0/5/5/5
3	F3V	B	302	-	-	0/1/2/2	-
3	F3V	P	302	-	-	0/1/2/2	-
3	F3V	H	302	-	-	0/1/2/2	-
2	NAP	B	301	-	-	3/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	E	301	-	-	1/35/67/67	0/5/5/5
3	F3V	K	302	-	-	0/1/2/2	-
3	F3V	C	302	-	-	0/1/2/2	-
3	F3V	D	302	-	-	0/1/2/2	-
3	F3V	G	302	-	-	0/1/2/2	-
3	F3V	F	302	-	-	0/1/2/2	-
3	F3V	L	302	-	-	0/1/2/2	-
2	NAP	D	301	-	-	3/35/67/67	0/5/5/5
2	NAP	G	301	-	-	2/35/67/67	0/5/5/5
2	NAP	F	301	-	-	4/35/67/67	0/5/5/5
2	NAP	O	301	5	-	2/35/67/67	0/5/5/5
3	F3V	N	302	-	-	0/1/2/2	-
2	NAP	P	301	-	-	5/35/67/67	0/5/5/5
3	F3V	M	302	-	-	0/1/2/2	-
2	NAP	K	301	-	-	4/35/67/67	0/5/5/5
2	NAP	C	301	5	-	4/35/67/67	0/5/5/5
2	NAP	M	301	-	-	7/35/67/67	0/5/5/5
2	NAP	I	301	-	-	1/35/67/67	0/5/5/5
2	NAP	H	301	5	-	2/35/67/67	0/5/5/5
3	F3V	I	302	-	-	0/1/2/2	-

All (309) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	C7N-N7N	9.59	1.50	1.33
2	G	301	NAP	C7N-N7N	9.34	1.50	1.33
2	N	301	NAP	C7N-N7N	9.19	1.49	1.33
2	J	301	NAP	C7N-N7N	9.18	1.49	1.33
2	M	301	NAP	C7N-N7N	9.17	1.49	1.33
2	B	301	NAP	C7N-N7N	9.15	1.49	1.33
2	O	301	NAP	C7N-N7N	9.07	1.49	1.33
2	L	301	NAP	C7N-N7N	9.06	1.49	1.33
2	I	301	NAP	C7N-N7N	9.02	1.49	1.33
2	E	301	NAP	C7N-N7N	8.98	1.49	1.33
2	P	301	NAP	C7N-N7N	8.98	1.49	1.33
2	F	301	NAP	C7N-N7N	8.92	1.49	1.33
2	K	301	NAP	C7N-N7N	8.83	1.49	1.33
2	A	301	NAP	C7N-N7N	8.81	1.49	1.33
2	H	301	NAP	C7N-N7N	8.52	1.48	1.33
2	C	301	NAP	C7N-N7N	8.40	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	O4D-C1D	7.97	1.51	1.40
2	A	301	NAP	O4D-C1D	7.74	1.51	1.40
2	F	301	NAP	O4D-C1D	7.73	1.51	1.40
2	D	301	NAP	O4D-C1D	7.68	1.51	1.40
2	K	301	NAP	O4D-C1D	7.63	1.50	1.40
2	N	301	NAP	O4D-C1D	7.60	1.50	1.40
2	E	301	NAP	O4D-C1D	7.60	1.50	1.40
2	P	301	NAP	O4D-C1D	7.50	1.50	1.40
2	M	301	NAP	O4D-C1D	7.50	1.50	1.40
2	L	301	NAP	O4D-C1D	7.48	1.50	1.40
2	I	301	NAP	O4D-C1D	7.33	1.50	1.40
2	O	301	NAP	O4D-C1D	7.30	1.50	1.40
2	J	301	NAP	O4D-C1D	7.22	1.50	1.40
2	G	301	NAP	O4D-C1D	7.08	1.50	1.40
2	C	301	NAP	O4D-C1D	6.94	1.50	1.40
2	G	301	NAP	PA-O3	6.81	1.66	1.59
2	O	301	NAP	PA-O3	6.79	1.66	1.59
2	H	301	NAP	O4D-C1D	6.70	1.49	1.40
2	M	301	NAP	PA-O3	6.09	1.66	1.59
2	B	301	NAP	C3N-C7N	6.07	1.59	1.50
2	D	301	NAP	PA-O3	5.99	1.66	1.59
2	L	301	NAP	PA-O3	5.90	1.65	1.59
2	M	301	NAP	C3N-C7N	5.81	1.59	1.50
2	I	301	NAP	PA-O3	5.79	1.65	1.59
2	K	301	NAP	C3N-C7N	5.68	1.59	1.50
2	K	301	NAP	PA-O3	5.65	1.65	1.59
2	N	301	NAP	C3N-C7N	5.64	1.59	1.50
2	J	301	NAP	PA-O3	5.61	1.65	1.59
2	N	301	NAP	PA-O3	5.60	1.65	1.59
2	B	301	NAP	PA-O3	5.53	1.65	1.59
2	L	301	NAP	C3N-C7N	5.51	1.58	1.50
2	H	301	NAP	P2B-O2B	5.49	1.69	1.59
2	A	301	NAP	C3N-C7N	5.44	1.58	1.50
2	I	301	NAP	C3N-C7N	5.40	1.58	1.50
2	M	301	NAP	P2B-O2B	5.39	1.69	1.59
2	F	301	NAP	P2B-O2B	5.36	1.68	1.59
2	L	301	NAP	P2B-O2B	5.36	1.68	1.59
2	A	301	NAP	PA-O3	5.34	1.65	1.59
2	H	301	NAP	C6A-N6A	5.29	1.47	1.34
2	O	301	NAP	C6A-N6A	5.28	1.47	1.34
2	J	301	NAP	P2B-O2B	5.27	1.68	1.59
2	B	301	NAP	P2B-O2B	5.26	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	301	NAP	PA-O3	5.22	1.65	1.59
2	J	301	NAP	C3N-C7N	5.17	1.58	1.50
2	J	301	NAP	C6A-N6A	5.16	1.47	1.34
2	P	301	NAP	C3N-C7N	5.16	1.58	1.50
2	A	301	NAP	P2B-O2B	5.08	1.68	1.59
2	P	301	NAP	P2B-O2B	5.05	1.68	1.59
2	I	301	NAP	C6A-N6A	5.04	1.47	1.34
2	N	301	NAP	C2N-N1N	5.03	1.40	1.35
2	F	301	NAP	C3N-C7N	4.98	1.58	1.50
2	B	301	NAP	C6A-N6A	4.97	1.46	1.34
2	E	301	NAP	P2B-O2B	4.96	1.68	1.59
2	H	301	NAP	C8A-N9A	-4.93	1.29	1.37
2	A	301	NAP	C6A-N6A	4.92	1.46	1.34
2	I	301	NAP	C8A-N9A	-4.91	1.29	1.37
2	L	301	NAP	C8A-N9A	-4.89	1.29	1.37
2	K	301	NAP	C6A-N6A	4.88	1.46	1.34
2	C	301	NAP	P2B-O2B	4.88	1.68	1.59
2	E	301	NAP	PA-O3	4.88	1.64	1.59
2	E	301	NAP	C3N-C7N	4.88	1.57	1.50
2	M	301	NAP	C6A-N6A	4.85	1.46	1.34
2	L	301	NAP	C6A-N6A	4.84	1.46	1.34
2	N	301	NAP	C6A-N6A	4.84	1.46	1.34
2	G	301	NAP	P2B-O2B	4.83	1.68	1.59
2	B	301	NAP	C8A-N9A	-4.83	1.29	1.37
2	O	301	NAP	C8A-N9A	-4.80	1.29	1.37
2	P	301	NAP	C6A-N6A	4.79	1.46	1.34
2	F	301	NAP	C6A-N6A	4.79	1.46	1.34
2	E	301	NAP	C6A-N6A	4.78	1.46	1.34
2	H	301	NAP	C3N-C7N	4.78	1.57	1.50
2	I	301	NAP	P2B-O2B	4.78	1.67	1.59
2	M	301	NAP	C8A-N9A	-4.77	1.29	1.37
2	K	301	NAP	P2B-O2B	4.77	1.67	1.59
2	E	301	NAP	C2N-N1N	4.76	1.40	1.35
2	A	301	NAP	C2N-N1N	4.76	1.40	1.35
2	G	301	NAP	C3N-C7N	4.74	1.57	1.50
2	G	301	NAP	C6A-N6A	4.74	1.46	1.34
2	N	301	NAP	P2B-O2B	4.72	1.67	1.59
2	C	301	NAP	C6A-N6A	4.68	1.46	1.34
2	O	301	NAP	PN-O3	4.67	1.64	1.59
2	B	301	NAP	C2N-N1N	4.66	1.40	1.35
2	N	301	NAP	C8A-N9A	-4.65	1.29	1.37
2	J	301	NAP	C8A-N9A	-4.65	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	301	NAP	C3N-C7N	4.62	1.57	1.50
2	I	301	NAP	C2N-N1N	4.59	1.40	1.35
2	E	301	NAP	C8A-N9A	-4.58	1.29	1.37
2	M	301	NAP	C2N-N1N	4.57	1.40	1.35
2	D	301	NAP	P2B-O2B	4.57	1.67	1.59
2	F	301	NAP	C8A-N9A	-4.56	1.29	1.37
2	P	301	NAP	C8A-N9A	-4.56	1.29	1.37
2	F	301	NAP	C2N-N1N	4.51	1.39	1.35
2	C	301	NAP	C2N-N1N	4.50	1.39	1.35
2	C	301	NAP	C3N-C7N	4.49	1.57	1.50
2	K	301	NAP	C8A-N9A	-4.47	1.29	1.37
2	P	301	NAP	C2N-N1N	4.47	1.39	1.35
2	C	301	NAP	C8A-N9A	-4.46	1.30	1.37
2	O	301	NAP	P2B-O2B	4.42	1.67	1.59
2	L	301	NAP	C2N-N1N	4.42	1.39	1.35
2	K	301	NAP	C2N-N1N	4.39	1.39	1.35
2	A	301	NAP	C8A-N9A	-4.38	1.30	1.37
2	J	301	NAP	C2N-N1N	4.33	1.39	1.35
2	H	301	NAP	PA-O3	4.31	1.64	1.59
2	D	301	NAP	C6A-N6A	4.27	1.45	1.34
2	D	301	NAP	C3N-C7N	4.25	1.56	1.50
2	F	301	NAP	PA-O3	4.23	1.64	1.59
2	H	301	NAP	C2N-N1N	4.23	1.39	1.35
2	G	301	NAP	C8A-N9A	-4.23	1.30	1.37
2	D	301	NAP	C2N-N1N	4.15	1.39	1.35
2	G	301	NAP	PN-O3	4.08	1.63	1.59
2	O	301	NAP	C2N-N1N	4.03	1.39	1.35
2	D	301	NAP	C8A-N9A	-3.89	1.30	1.37
2	D	301	NAP	C4A-N9A	-3.89	1.29	1.37
2	E	301	NAP	PN-O3	3.86	1.63	1.59
2	M	301	NAP	PN-O3	3.85	1.63	1.59
2	G	301	NAP	C2N-N1N	3.83	1.39	1.35
2	G	301	NAP	C4A-N9A	-3.82	1.29	1.37
2	F	301	NAP	C4A-N9A	-3.81	1.29	1.37
2	D	301	NAP	PN-O3	3.81	1.63	1.59
2	M	301	NAP	C4A-N9A	-3.70	1.30	1.37
2	A	301	NAP	C4A-N9A	-3.69	1.30	1.37
2	K	301	NAP	C4A-N9A	-3.64	1.30	1.37
2	N	301	NAP	PN-O3	3.64	1.63	1.59
2	I	301	NAP	PN-O3	3.57	1.63	1.59
2	C	301	NAP	C4A-N9A	-3.57	1.30	1.37
2	N	301	NAP	C4A-N9A	-3.53	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	NAP	PN-O3	3.52	1.63	1.59
2	H	301	NAP	C4A-N9A	-3.52	1.30	1.37
2	J	301	NAP	C4A-N9A	-3.48	1.30	1.37
2	I	301	NAP	C4A-N9A	-3.43	1.30	1.37
2	B	301	NAP	O4D-C4D	3.42	1.52	1.45
2	J	301	NAP	PN-O3	3.41	1.63	1.59
2	L	301	NAP	C4A-N9A	-3.40	1.30	1.37
2	B	301	NAP	C4A-N9A	-3.39	1.30	1.37
2	P	301	NAP	C4A-N9A	-3.36	1.30	1.37
2	E	301	NAP	O4D-C4D	3.36	1.52	1.45
2	N	301	NAP	O4D-C4D	3.31	1.52	1.45
2	M	301	NAP	O4D-C4D	3.27	1.52	1.45
2	K	301	NAP	O4D-C4D	3.27	1.52	1.45
2	O	301	NAP	C4A-N9A	-3.27	1.30	1.37
2	B	301	NAP	PN-O3	3.22	1.63	1.59
2	L	301	NAP	PN-O3	3.17	1.62	1.59
2	G	301	NAP	O4B-C4B	3.16	1.52	1.45
2	L	301	NAP	O4D-C4D	3.16	1.52	1.45
2	N	301	NAP	C2N-C3N	3.15	1.44	1.39
2	J	301	NAP	O4D-C4D	3.13	1.52	1.45
2	C	301	NAP	PA-O3	3.13	1.62	1.59
2	D	301	NAP	O4B-C4B	3.09	1.51	1.45
2	D	301	NAP	O4D-C4D	3.07	1.51	1.45
2	E	301	NAP	C4A-N9A	-3.07	1.31	1.37
2	A	301	NAP	O4B-C4B	3.07	1.51	1.45
2	E	301	NAP	C3B-C2B	-3.05	1.46	1.53
2	N	301	NAP	C3B-C2B	-3.05	1.46	1.53
2	P	301	NAP	O4B-C4B	3.04	1.51	1.45
2	P	301	NAP	O4D-C4D	3.03	1.51	1.45
2	K	301	NAP	O4B-C4B	3.01	1.51	1.45
2	I	301	NAP	C2N-C3N	3.01	1.43	1.39
2	M	301	NAP	O4B-C4B	3.01	1.51	1.45
2	G	301	NAP	C3B-C2B	-3.00	1.46	1.53
2	I	301	NAP	O4B-C4B	2.99	1.51	1.45
2	H	301	NAP	C2N-C3N	2.99	1.43	1.39
2	D	301	NAP	C3B-C2B	-2.99	1.46	1.53
2	F	301	NAP	C3D-C4D	-2.98	1.45	1.53
2	M	301	NAP	O4B-C1B	2.98	1.48	1.42
2	G	301	NAP	O4D-C4D	2.97	1.51	1.45
2	O	301	NAP	O4D-C4D	2.96	1.51	1.45
2	F	301	NAP	O4B-C1B	2.96	1.48	1.42
2	M	301	NAP	C3D-C4D	-2.96	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	NAP	C3B-C2B	-2.94	1.46	1.53
2	J	301	NAP	C2N-C3N	2.94	1.43	1.39
2	L	301	NAP	O4B-C1B	2.94	1.48	1.42
2	F	301	NAP	C2N-C3N	2.92	1.43	1.39
2	N	301	NAP	O4B-C4B	2.92	1.51	1.45
2	O	301	NAP	O4B-C4B	2.91	1.51	1.45
2	I	301	NAP	O4D-C4D	2.91	1.51	1.45
2	I	301	NAP	O4B-C1B	2.89	1.48	1.42
2	N	301	NAP	O4B-C1B	2.88	1.48	1.42
2	B	301	NAP	O4B-C4B	2.88	1.51	1.45
2	E	301	NAP	O4B-C1B	2.87	1.48	1.42
2	E	301	NAP	O4B-C4B	2.87	1.51	1.45
2	L	301	NAP	O4B-C4B	2.85	1.51	1.45
2	J	301	NAP	O4B-C4B	2.85	1.51	1.45
2	E	301	NAP	C2N-C3N	2.85	1.43	1.39
2	B	301	NAP	C3B-C2B	-2.85	1.46	1.53
2	G	301	NAP	C3D-C4D	-2.85	1.45	1.53
2	K	301	NAP	C3D-C4D	-2.84	1.45	1.53
2	H	301	NAP	O4D-C4D	2.82	1.51	1.45
2	K	301	NAP	O4B-C1B	2.82	1.48	1.42
2	O	301	NAP	C3B-C2B	-2.81	1.46	1.53
2	L	301	NAP	C2N-C3N	2.80	1.43	1.39
2	K	301	NAP	C2N-C3N	2.79	1.43	1.39
2	F	301	NAP	C3B-C2B	-2.79	1.46	1.53
2	C	301	NAP	O4D-C4D	2.79	1.51	1.45
2	A	301	NAP	O4D-C4D	2.78	1.51	1.45
2	M	301	NAP	C2N-C3N	2.78	1.43	1.39
2	A	301	NAP	C3D-C4D	-2.78	1.45	1.53
2	I	301	NAP	C3B-C2B	-2.77	1.46	1.53
2	P	301	NAP	C3D-C4D	-2.76	1.46	1.53
2	B	301	NAP	C2N-C3N	2.76	1.43	1.39
2	A	301	NAP	O4B-C1B	2.76	1.48	1.42
2	L	301	NAP	C3D-C4D	-2.75	1.46	1.53
2	J	301	NAP	O4B-C1B	2.74	1.48	1.42
2	D	301	NAP	O4B-C1B	2.74	1.48	1.42
2	I	301	NAP	C2D-C3D	-2.73	1.46	1.53
2	P	301	NAP	O4B-C1B	2.72	1.48	1.42
2	F	301	NAP	O4D-C4D	2.70	1.51	1.45
2	H	301	NAP	O4B-C4B	2.68	1.51	1.45
2	P	301	NAP	C2D-C3D	-2.68	1.46	1.53
2	F	301	NAP	PN-O3	2.68	1.62	1.59
2	B	301	NAP	C3D-C4D	-2.67	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAP	C2N-C3N	2.67	1.43	1.39
2	B	301	NAP	O4B-C1B	2.66	1.48	1.42
2	E	301	NAP	C3D-C4D	-2.66	1.46	1.53
2	F	301	NAP	O4B-C4B	2.65	1.50	1.45
2	G	301	NAP	O4B-C1B	2.64	1.48	1.42
2	P	301	NAP	C2N-C3N	2.62	1.43	1.39
2	M	301	NAP	C2D-C3D	-2.62	1.46	1.53
2	A	301	NAP	C3B-C2B	-2.62	1.47	1.53
2	M	301	NAP	C3B-C2B	-2.61	1.47	1.53
2	K	301	NAP	C2D-C3D	-2.60	1.46	1.53
2	D	301	NAP	C2D-C3D	-2.59	1.46	1.53
2	P	301	NAP	C3B-C2B	-2.58	1.47	1.53
2	N	301	NAP	C3D-C4D	-2.58	1.46	1.53
2	L	301	NAP	C3B-C2B	-2.57	1.47	1.53
2	D	301	NAP	C3D-C4D	-2.55	1.46	1.53
2	C	301	NAP	C3B-C2B	-2.55	1.47	1.53
2	C	301	NAP	C2D-C3D	-2.55	1.46	1.53
2	I	301	NAP	C3D-C4D	-2.54	1.46	1.53
2	A	301	NAP	PN-O3	2.54	1.62	1.59
2	H	301	NAP	O4B-C1B	2.53	1.47	1.42
2	A	301	NAP	C2N-C3N	2.48	1.42	1.39
2	B	301	NAP	C2D-C3D	-2.47	1.46	1.53
2	N	301	NAP	C2D-C3D	-2.46	1.46	1.53
2	C	301	NAP	O4B-C4B	2.45	1.50	1.45
2	O	301	NAP	O4B-C1B	2.43	1.47	1.42
2	O	301	NAP	C2D-C3D	-2.43	1.46	1.53
2	H	301	NAP	C2D-C3D	-2.41	1.46	1.53
2	P	301	NAP	PN-O3	2.41	1.62	1.59
2	J	301	NAP	C3B-C2B	-2.40	1.47	1.53
2	J	301	NAP	C2D-C3D	-2.40	1.46	1.53
2	J	301	NAP	C3D-C4D	-2.35	1.47	1.53
2	E	301	NAP	C2D-C3D	-2.35	1.47	1.53
2	I	301	NAP	O3D-C3D	2.34	1.48	1.43
2	H	301	NAP	C3B-C2B	-2.33	1.47	1.53
2	L	301	NAP	C2D-C3D	-2.32	1.47	1.53
2	A	301	NAP	C5A-C4A	2.32	1.43	1.39
2	B	301	NAP	C5A-C4A	2.29	1.43	1.39
2	P	301	NAP	C3B-C4B	-2.28	1.47	1.53
2	C	301	NAP	O4B-C1B	2.28	1.47	1.42
2	O	301	NAP	C3D-C4D	-2.27	1.47	1.53
2	O	301	NAP	C2N-C3N	2.26	1.42	1.39
2	F	301	NAP	C5A-C4A	2.26	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	NAP	C3B-C4B	-2.24	1.47	1.53
2	G	301	NAP	C2D-C3D	-2.24	1.47	1.53
2	H	301	NAP	C5A-C4A	2.23	1.43	1.39
2	J	301	NAP	O3D-C3D	2.22	1.48	1.43
2	A	301	NAP	O3D-C3D	2.19	1.48	1.43
2	K	301	NAP	C3B-C4B	-2.19	1.47	1.53
2	M	301	NAP	PA-O5B	2.17	1.67	1.59
2	N	301	NAP	C5A-C4A	2.15	1.42	1.39
2	H	301	NAP	C3D-C4D	-2.14	1.47	1.53
2	G	301	NAP	O3D-C3D	2.14	1.48	1.43
2	I	301	NAP	C5A-C4A	2.14	1.42	1.39
2	N	301	NAP	C3B-C4B	-2.13	1.47	1.53
2	O	301	NAP	C3B-C4B	-2.13	1.47	1.53
2	J	301	NAP	C3B-C4B	-2.13	1.47	1.53
2	L	301	NAP	C3B-C4B	-2.12	1.47	1.53
2	E	301	NAP	C5A-C4A	2.12	1.42	1.39
2	A	301	NAP	C3B-C4B	-2.12	1.47	1.53
2	F	301	NAP	C3B-C4B	-2.11	1.47	1.53
2	G	301	NAP	C2N-C3N	2.10	1.42	1.39
2	O	301	NAP	O3D-C3D	2.10	1.48	1.43
2	I	301	NAP	C3B-C4B	-2.10	1.47	1.53
2	L	301	NAP	PA-O5B	2.10	1.67	1.59
2	C	301	NAP	C3B-C4B	-2.09	1.47	1.53
2	B	301	NAP	C6N-C5N	2.09	1.43	1.38
2	K	301	NAP	O3D-C3D	2.09	1.48	1.43
2	B	301	NAP	C3B-C4B	-2.09	1.47	1.53
2	E	301	NAP	C6N-C5N	2.08	1.42	1.38
2	D	301	NAP	C2N-C3N	2.07	1.42	1.39
2	H	301	NAP	O3D-C3D	2.07	1.48	1.43
2	F	301	NAP	C2D-C3D	-2.06	1.47	1.53
2	J	301	NAP	PA-O5B	2.05	1.67	1.59
2	K	301	NAP	C5A-C4A	2.05	1.42	1.39
2	D	301	NAP	C3B-C4B	-2.05	1.47	1.53
2	E	301	NAP	O3D-C3D	2.04	1.48	1.43
2	N	301	NAP	PA-O5B	2.04	1.67	1.59
2	P	301	NAP	O3D-C3D	2.03	1.48	1.43
2	P	301	NAP	C5A-C4A	2.02	1.42	1.39
2	L	301	NAP	C5A-C4A	2.01	1.42	1.39
2	M	301	NAP	C3B-C4B	-2.01	1.47	1.53
2	F	301	NAP	PA-O5B	2.01	1.67	1.59
2	C	301	NAP	C5A-C4A	2.00	1.42	1.39

All (278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	NAP	C4A-N9A-C8A	9.50	115.72	105.74
2	B	301	NAP	C4A-N9A-C8A	9.12	115.31	105.74
2	G	301	NAP	C4A-N9A-C8A	9.11	115.30	105.74
2	K	301	NAP	C4A-N9A-C8A	8.94	115.12	105.74
2	P	301	NAP	C4A-N9A-C8A	8.87	115.05	105.74
2	N	301	NAP	C4A-N9A-C8A	8.85	115.03	105.74
2	M	301	NAP	C4A-N9A-C8A	8.84	115.03	105.74
2	O	301	NAP	C4A-N9A-C8A	8.80	114.98	105.74
2	L	301	NAP	C4A-N9A-C8A	8.66	114.83	105.74
2	C	301	NAP	C4A-N9A-C8A	8.64	114.81	105.74
2	J	301	NAP	C4A-N9A-C8A	8.61	114.78	105.74
2	F	301	NAP	C4A-N9A-C8A	8.59	114.76	105.74
2	A	301	NAP	C4A-N9A-C8A	8.56	114.73	105.74
2	O	301	NAP	C4D-O4D-C1D	-8.50	102.14	109.92
2	D	301	NAP	C4A-N9A-C8A	8.44	114.61	105.74
2	D	301	NAP	C4D-O4D-C1D	-8.40	102.23	109.92
2	I	301	NAP	C4A-N9A-C8A	8.31	114.46	105.74
2	G	301	NAP	C4D-O4D-C1D	-8.14	102.47	109.92
2	E	301	NAP	C4A-N9A-C8A	8.06	114.20	105.74
2	K	301	NAP	C4D-O4D-C1D	-7.78	102.80	109.92
2	P	301	NAP	C4D-O4D-C1D	-7.69	102.89	109.92
2	I	301	NAP	C4D-O4D-C1D	-7.41	103.14	109.92
2	L	301	NAP	C4D-O4D-C1D	-7.33	103.22	109.92
2	M	301	NAP	C4D-O4D-C1D	-7.32	103.22	109.92
2	A	301	NAP	C4D-O4D-C1D	-6.95	103.56	109.92
2	J	301	NAP	C4D-O4D-C1D	-6.70	103.79	109.92
2	H	301	NAP	C4D-O4D-C1D	-6.63	103.86	109.92
2	B	301	NAP	C4D-O4D-C1D	-6.45	104.02	109.92
2	F	301	NAP	C4D-O4D-C1D	-6.35	104.11	109.92
2	N	301	NAP	C4D-O4D-C1D	-6.30	104.16	109.92
2	E	301	NAP	C5A-C4A-N3A	-6.08	118.35	126.72
2	C	301	NAP	C4D-O4D-C1D	-5.99	104.44	109.92
2	E	301	NAP	N3A-C4A-N9A	5.96	137.30	127.17
2	E	301	NAP	C4D-O4D-C1D	-5.93	104.50	109.92
2	C	301	NAP	N3A-C2A-N1A	-5.89	119.66	128.58
2	P	301	NAP	N3A-C4A-N9A	5.86	137.12	127.17
2	O	301	NAP	N3A-C4A-N9A	5.85	137.11	127.17
2	B	301	NAP	N3A-C4A-N9A	5.79	137.01	127.17
2	L	301	NAP	N3A-C4A-N9A	5.72	136.89	127.17
2	O	301	NAP	C5A-C4A-N3A	-5.68	118.89	126.72
2	N	301	NAP	N3A-C4A-N9A	5.56	136.63	127.17
2	L	301	NAP	C5A-C4A-N3A	-5.55	119.08	126.72
2	P	301	NAP	C5A-C4A-N3A	-5.54	119.08	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	301	NAP	N3A-C4A-N9A	5.51	136.54	127.17
2	J	301	NAP	N3A-C4A-N9A	5.46	136.46	127.17
2	K	301	NAP	N3A-C4A-N9A	5.45	136.43	127.17
2	I	301	NAP	N3A-C4A-N9A	5.44	136.42	127.17
2	F	301	NAP	C5A-C4A-N3A	-5.43	119.25	126.72
2	G	301	NAP	N3A-C4A-N9A	5.42	136.38	127.17
2	D	301	NAP	N3A-C4A-N9A	5.38	136.32	127.17
2	F	301	NAP	N3A-C4A-N9A	5.38	136.31	127.17
2	N	301	NAP	C5A-C4A-N3A	-5.37	119.32	126.72
2	H	301	NAP	N3A-C4A-N9A	5.37	136.30	127.17
2	I	301	NAP	C5A-C4A-N3A	-5.32	119.39	126.72
2	D	301	NAP	C5A-C4A-N3A	-5.28	119.44	126.72
2	J	301	NAP	C5A-C4A-N3A	-5.28	119.45	126.72
2	B	301	NAP	C5A-C4A-N3A	-5.27	119.46	126.72
2	H	301	NAP	C5A-C4A-N3A	-5.22	119.52	126.72
2	A	301	NAP	C5A-C4A-N3A	-5.22	119.53	126.72
2	M	301	NAP	C5A-C4A-N3A	-5.21	119.54	126.72
2	C	301	NAP	C5A-C4A-N3A	-5.12	119.67	126.72
2	K	301	NAP	C5A-C4A-N3A	-5.05	119.76	126.72
2	G	301	NAP	C5A-C4A-N3A	-5.05	119.76	126.72
2	A	301	NAP	N3A-C4A-N9A	5.02	135.70	127.17
2	C	301	NAP	N3A-C4A-N9A	4.96	135.61	127.17
2	A	301	NAP	C4A-C5A-N7A	-4.80	105.09	110.58
2	H	301	NAP	C4A-C5A-N7A	-4.80	105.10	110.58
2	H	301	NAP	N9A-C8A-N7A	-4.74	107.22	113.94
2	G	301	NAP	N9A-C8A-N7A	-4.69	107.29	113.94
2	O	301	NAP	C4A-C5A-N7A	-4.62	105.30	110.58
2	I	301	NAP	C4A-C5A-N7A	-4.60	105.33	110.58
2	N	301	NAP	C4A-C5A-N7A	-4.59	105.33	110.58
2	D	301	NAP	N3A-C2A-N1A	-4.58	121.65	128.58
2	E	301	NAP	C4A-C5A-N7A	-4.54	105.39	110.58
2	F	301	NAP	C4A-C5A-N7A	-4.53	105.40	110.58
2	O	301	NAP	N9A-C8A-N7A	-4.53	107.51	113.94
2	D	301	NAP	N9A-C8A-N7A	-4.51	107.54	113.94
2	A	301	NAP	N3A-C2A-N1A	-4.46	121.83	128.58
2	L	301	NAP	C4A-C5A-N7A	-4.44	105.50	110.58
2	B	301	NAP	C4A-C5A-N7A	-4.43	105.52	110.58
2	B	301	NAP	N9A-C8A-N7A	-4.40	107.70	113.94
2	J	301	NAP	C4A-C5A-N7A	-4.39	105.56	110.58
2	E	301	NAP	N3A-C2A-N1A	-4.39	121.94	128.58
2	C	301	NAP	N9A-C8A-N7A	-4.38	107.72	113.94
2	K	301	NAP	N9A-C8A-N7A	-4.34	107.78	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	301	NAP	N9A-C8A-N7A	-4.34	107.78	113.94
2	K	301	NAP	N3A-C2A-N1A	-4.34	122.02	128.58
2	J	301	NAP	N9A-C8A-N7A	-4.29	107.85	113.94
2	F	301	NAP	N3A-C2A-N1A	-4.29	122.09	128.58
2	C	301	NAP	C4A-C5A-N7A	-4.28	105.69	110.58
2	N	301	NAP	N3A-C2A-N1A	-4.27	122.11	128.58
2	L	301	NAP	N9A-C8A-N7A	-4.27	107.88	113.94
2	P	301	NAP	N9A-C8A-N7A	-4.25	107.90	113.94
2	I	301	NAP	N3A-C2A-N1A	-4.25	122.16	128.58
2	M	301	NAP	N9A-C8A-N7A	-4.24	107.92	113.94
2	O	301	NAP	N3A-C2A-N1A	-4.24	122.17	128.58
2	M	301	NAP	C4A-C5A-N7A	-4.23	105.75	110.58
2	H	301	NAP	N3A-C2A-N1A	-4.22	122.20	128.58
2	K	301	NAP	C4A-C5A-N7A	-4.19	105.79	110.58
2	L	301	NAP	N3A-C2A-N1A	-4.17	122.26	128.58
2	P	301	NAP	C4A-C5A-N7A	-4.17	105.81	110.58
2	J	301	NAP	N3A-C2A-N1A	-4.14	122.32	128.58
2	A	301	NAP	N9A-C8A-N7A	-4.13	108.08	113.94
2	P	301	NAP	N3A-C2A-N1A	-4.12	122.34	128.58
2	G	301	NAP	C4A-C5A-N7A	-4.12	105.87	110.58
2	M	301	NAP	N3A-C2A-N1A	-4.11	122.35	128.58
2	F	301	NAP	N9A-C8A-N7A	-4.10	108.12	113.94
2	C	301	NAP	C2A-N3A-C4A	4.05	121.73	111.83
2	I	301	NAP	N9A-C8A-N7A	-3.97	108.30	113.94
2	B	301	NAP	N3A-C2A-N1A	-3.93	122.63	128.58
2	G	301	NAP	N3A-C2A-N1A	-3.89	122.69	128.58
2	E	301	NAP	N9A-C8A-N7A	-3.84	108.48	113.94
3	B	302	F3V	CM-C-CA	3.79	121.04	115.47
2	E	301	NAP	C2A-N3A-C4A	3.79	121.09	111.83
3	I	302	F3V	CM-C-CA	3.78	121.02	115.47
2	D	301	NAP	C4A-C5A-N7A	-3.59	106.47	110.58
2	D	301	NAP	C2A-N3A-C4A	3.56	120.53	111.83
3	B	302	F3V	O-C-CA	-3.55	118.61	121.28
2	A	301	NAP	C2A-N3A-C4A	3.55	120.50	111.83
2	F	301	NAP	C2A-N3A-C4A	3.53	120.46	111.83
3	H	302	F3V	CM-C-CA	3.51	120.63	115.47
3	E	302	F3V	CM-C-CA	3.50	120.61	115.47
2	N	301	NAP	C2A-N3A-C4A	3.48	120.33	111.83
2	L	301	NAP	C2A-N3A-C4A	3.47	120.31	111.83
2	P	301	NAP	C2A-N3A-C4A	3.44	120.24	111.83
3	M	302	F3V	CM-C-CA	3.43	120.51	115.47
2	O	301	NAP	C2A-N3A-C4A	3.41	120.16	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	302	F3V	CM-C-CA	3.35	120.39	115.47
2	K	301	NAP	C2A-N3A-C4A	3.34	120.00	111.83
2	J	301	NAP	C2A-N3A-C4A	3.34	119.99	111.83
2	I	301	NAP	C2A-N3A-C4A	3.31	119.92	111.83
2	M	301	NAP	C2A-N3A-C4A	3.27	119.82	111.83
3	A	302	F3V	CM-C-CA	3.22	120.20	115.47
2	E	301	NAP	O2N-PN-O3	3.18	115.88	107.27
2	B	301	NAP	C2A-N3A-C4A	3.18	119.60	111.83
2	G	301	NAP	C2A-N3A-C4A	3.17	119.58	111.83
2	H	301	NAP	C2A-N3A-C4A	3.17	119.56	111.83
2	D	301	NAP	C3N-C7N-N7N	3.16	121.64	117.74
3	L	302	F3V	CM-C-CA	3.14	120.08	115.47
3	P	302	F3V	CM-C-CA	3.13	120.07	115.47
3	N	302	F3V	CM-C-CA	3.09	120.01	115.47
2	O	301	NAP	C5A-N7A-C8A	3.03	108.21	103.45
3	O	302	F3V	CM-C-CA	3.03	119.92	115.47
3	I	302	F3V	O-C-CA	-2.97	119.04	121.28
2	A	301	NAP	C4A-N9A-C1B	-2.95	119.74	126.63
2	E	301	NAP	C6N-N1N-C2N	-2.91	119.40	121.88
2	C	301	NAP	C6A-C5A-N7A	2.86	137.61	132.09
2	B	301	NAP	C5A-N7A-C8A	2.85	107.94	103.45
2	I	301	NAP	P2B-O2B-C2B	-2.84	115.85	123.43
2	F	301	NAP	C2D-C3D-C4D	2.83	108.07	102.61
3	F	302	F3V	CM-C-CA	2.81	119.61	115.47
2	K	301	NAP	C4A-N9A-C1B	-2.81	120.06	126.63
2	C	301	NAP	C4A-N9A-C1B	-2.81	120.06	126.63
2	N	301	NAP	C5A-N7A-C8A	2.77	107.81	103.45
2	N	301	NAP	C3N-C7N-N7N	2.76	121.14	117.74
2	H	301	NAP	C5A-N7A-C8A	2.76	107.79	103.45
2	N	301	NAP	C6N-N1N-C2N	-2.76	119.53	121.88
3	G	302	F3V	CM-C-CA	2.75	119.50	115.47
2	L	301	NAP	C5A-N7A-C8A	2.73	107.75	103.45
2	G	301	NAP	C4A-N9A-C1B	-2.73	120.25	126.63
2	H	301	NAP	C2D-C3D-C4D	2.72	107.87	102.61
2	I	301	NAP	C5A-N7A-C8A	2.72	107.73	103.45
2	N	301	NAP	C2D-C3D-C4D	2.72	107.86	102.61
2	A	301	NAP	C6A-C5A-N7A	2.71	137.31	132.09
2	J	301	NAP	C5A-N7A-C8A	2.71	107.70	103.45
2	G	301	NAP	C5A-N7A-C8A	2.69	107.68	103.45
2	E	301	NAP	C2N-C3N-C4N	2.68	121.37	118.26
2	B	301	NAP	O3D-C3D-C4D	-2.66	103.44	111.08
2	F	301	NAP	O3D-C3D-C4D	-2.66	103.44	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	C4A-N9A-C1B	-2.65	120.42	126.63
2	O	301	NAP	P2B-O2B-C2B	-2.64	116.38	123.43
3	J	302	F3V	CM-C-CA	2.64	119.35	115.47
2	N	301	NAP	C4A-N9A-C1B	-2.64	120.47	126.63
2	E	301	NAP	C5A-N7A-C8A	2.62	107.57	103.45
2	H	301	NAP	C4B-O4B-C1B	-2.62	103.68	109.47
2	J	301	NAP	C6N-N1N-C2N	-2.61	119.65	121.88
2	F	301	NAP	C4A-N9A-C1B	-2.61	120.53	126.63
2	L	301	NAP	C2D-C3D-C4D	2.60	107.63	102.61
2	K	301	NAP	C5A-N7A-C8A	2.58	107.50	103.45
2	N	301	NAP	C6A-C5A-N7A	2.58	137.06	132.09
2	L	301	NAP	C6N-N1N-C2N	-2.58	119.69	121.88
2	L	301	NAP	C4B-O4B-C1B	-2.57	103.78	109.47
2	F	301	NAP	C6A-C5A-N7A	2.56	137.03	132.09
2	P	301	NAP	C5A-N7A-C8A	2.54	107.45	103.45
2	E	301	NAP	C2D-C3D-C4D	2.53	107.50	102.61
2	C	301	NAP	O3D-C3D-C4D	-2.52	103.84	111.08
2	K	301	NAP	C4B-O4B-C1B	-2.51	103.92	109.47
2	M	301	NAP	C5A-N7A-C8A	2.51	107.39	103.45
2	F	301	NAP	C4B-O4B-C1B	-2.51	103.93	109.47
2	F	301	NAP	O2N-PN-O3	2.50	114.04	107.27
2	O	301	NAP	C2D-C3D-C4D	2.50	107.44	102.61
2	J	301	NAP	C3N-C7N-N7N	2.50	120.82	117.74
2	J	301	NAP	C4A-N9A-C1B	-2.49	120.80	126.63
2	L	301	NAP	C4A-N9A-C1B	-2.49	120.81	126.63
3	H	302	F3V	O-C-CA	-2.48	119.41	121.28
2	A	301	NAP	C5A-N7A-C8A	2.47	107.33	103.45
2	B	301	NAP	O2N-PN-O3	2.46	113.94	107.27
2	J	301	NAP	C2D-C3D-C4D	2.46	107.37	102.61
2	H	301	NAP	C6N-N1N-C2N	-2.45	119.79	121.88
2	N	301	NAP	C4B-O4B-C1B	-2.45	104.06	109.47
2	M	301	NAP	C4A-N9A-C1B	-2.44	120.92	126.63
2	F	301	NAP	C5A-N7A-C8A	2.44	107.28	103.45
2	C	301	NAP	C2D-C3D-C4D	2.43	107.31	102.61
2	H	301	NAP	C2N-C3N-C4N	2.43	121.09	118.26
2	B	301	NAP	C4B-O4B-C1B	-2.43	104.10	109.47
2	F	301	NAP	C6N-N1N-C2N	-2.42	119.82	121.88
2	C	301	NAP	C2A-N1A-C6A	2.42	122.70	118.73
2	G	301	NAP	P2B-O2B-C2B	-2.41	117.00	123.43
2	K	301	NAP	C6A-C5A-N7A	2.40	136.72	132.09
3	C	302	F3V	CM-C-CA	2.38	118.97	115.47
2	J	301	NAP	C2N-C3N-C4N	2.38	121.03	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	P2B-O2B-C2B	-2.37	117.09	123.43
2	L	301	NAP	C6A-C5A-N7A	2.37	136.65	132.09
2	I	301	NAP	C4B-O4B-C1B	-2.37	104.24	109.47
2	P	301	NAP	C4A-N9A-C1B	-2.35	121.14	126.63
2	D	301	NAP	C5A-N7A-C8A	2.35	107.14	103.45
2	K	301	NAP	P2B-O2B-C2B	-2.34	117.18	123.43
2	I	301	NAP	C6A-C5A-N7A	2.34	136.60	132.09
2	O	301	NAP	C2N-C3N-C4N	2.34	120.98	118.26
2	K	301	NAP	C6N-N1N-C2N	-2.33	119.89	121.88
2	F	301	NAP	C3N-C7N-N7N	2.32	120.60	117.74
2	M	301	NAP	O3D-C3D-C4D	-2.31	104.45	111.08
2	C	301	NAP	C5A-N7A-C8A	2.30	107.07	103.45
2	B	301	NAP	C3N-C7N-N7N	2.29	120.56	117.74
2	I	301	NAP	C2D-C3D-C4D	2.29	107.03	102.61
2	A	301	NAP	O3D-C3D-C4D	-2.28	104.53	111.08
2	E	301	NAP	C6A-C5A-N7A	2.26	136.45	132.09
2	H	301	NAP	C4A-N9A-C1B	-2.24	121.41	126.63
2	B	301	NAP	C4A-N9A-C1B	-2.23	121.41	126.63
2	H	301	NAP	C6A-C5A-N7A	2.23	136.39	132.09
2	J	301	NAP	C6A-C5A-N7A	2.23	136.39	132.09
2	D	301	NAP	C5B-C4B-C3B	-2.22	107.20	115.21
2	M	301	NAP	C6A-C5A-N7A	2.22	136.38	132.09
2	I	301	NAP	C4A-N9A-C1B	-2.22	121.44	126.63
2	D	301	NAP	C2D-C3D-C4D	2.21	106.89	102.61
2	G	301	NAP	C6A-C5A-N7A	2.21	136.35	132.09
2	A	301	NAP	C3N-C7N-N7N	2.20	120.45	117.74
2	M	301	NAP	C4B-O4B-C1B	-2.20	104.61	109.47
2	F	301	NAP	C2B-C3B-C4B	2.20	106.72	101.99
2	I	301	NAP	C3N-C7N-N7N	2.20	120.44	117.74
2	B	301	NAP	C6A-C5A-N7A	2.20	136.32	132.09
2	B	301	NAP	O7N-C7N-N7N	-2.19	119.46	122.62
2	M	301	NAP	C3N-C7N-N7N	2.18	120.42	117.74
2	M	301	NAP	C2D-C3D-C4D	2.17	106.80	102.61
2	H	301	NAP	C5N-C4N-C3N	-2.16	118.24	120.36
2	A	301	NAP	O2N-PN-O3	2.16	113.10	107.27
2	P	301	NAP	C4B-O4B-C1B	-2.16	104.71	109.47
2	E	301	NAP	O4B-C1B-N9A	2.14	112.20	108.09
2	G	301	NAP	C4B-O4B-C1B	-2.14	104.75	109.47
2	E	301	NAP	C4B-O4B-C1B	-2.13	104.77	109.47
2	G	301	NAP	C2D-C3D-C4D	2.12	106.70	102.61
2	K	301	NAP	O2N-PN-O3	2.11	112.99	107.27
2	P	301	NAP	C6A-C5A-N7A	2.11	136.16	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	301	NAP	C6N-N1N-C2N	-2.11	120.08	121.88
2	B	301	NAP	C2D-C3D-C4D	2.11	106.68	102.61
2	D	301	NAP	O7N-C7N-C3N	-2.10	117.03	119.60
2	I	301	NAP	C6N-N1N-C2N	-2.09	120.09	121.88
2	G	301	NAP	O3D-C3D-C4D	-2.09	105.07	111.08
2	B	301	NAP	C5A-C4A-N9A	-2.09	103.53	105.81
2	P	301	NAP	C2D-C3D-C4D	2.09	106.65	102.61
2	A	301	NAP	C2D-C3D-C4D	2.09	106.64	102.61
2	O	301	NAP	C6A-C5A-N7A	2.08	136.11	132.09
2	B	301	NAP	C6N-N1N-C2N	-2.08	120.11	121.88
2	M	301	NAP	C2B-C3B-C4B	2.08	106.47	101.99
2	O	301	NAP	C4B-O4B-C1B	-2.08	104.88	109.47
2	B	301	NAP	P2B-O2B-C2B	-2.08	117.89	123.43
2	L	301	NAP	C2B-C3B-C4B	2.07	106.45	101.99
2	A	301	NAP	C4B-O4B-C1B	-2.07	104.89	109.47
2	I	301	NAP	C2A-N1A-C6A	2.06	122.12	118.73
2	N	301	NAP	O2N-PN-O3	2.06	112.84	107.27
2	D	301	NAP	O3D-C3D-C4D	-2.05	105.18	111.08
2	C	301	NAP	O3X-P2B-O2X	2.04	115.45	107.80
2	D	301	NAP	O2N-PN-O3	2.04	112.78	107.27
2	O	301	NAP	C1B-N9A-C8A	-2.04	122.58	127.09
2	K	301	NAP	O3D-C3D-C4D	-2.02	105.27	111.08
2	D	301	NAP	C6A-C5A-N7A	2.02	135.99	132.09
2	P	301	NAP	C2B-C3B-C4B	2.00	106.30	101.99
2	E	301	NAP	O3D-C3D-C4D	-2.00	105.33	111.08

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	301	NAP	C5B-O5B-PA-O3
2	A	301	NAP	O4D-C4D-C5D-O5D
2	K	301	NAP	O4D-C4D-C5D-O5D
2	M	301	NAP	O4D-C4D-C5D-O5D
2	A	301	NAP	C3D-C4D-C5D-O5D
2	P	301	NAP	O4D-C4D-C5D-O5D
2	A	301	NAP	C2B-O2B-P2B-O2X
2	L	301	NAP	C2B-O2B-P2B-O2X
2	N	301	NAP	C2B-O2B-P2B-O2X
2	D	301	NAP	O4D-C4D-C5D-O5D
2	G	301	NAP	O4D-C4D-C5D-O5D
2	M	301	NAP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	M	301	NAP	C3D-C4D-C5D-O5D
2	B	301	NAP	C2B-O2B-P2B-O2X
2	F	301	NAP	C2B-O2B-P2B-O2X
2	P	301	NAP	C2B-O2B-P2B-O2X
2	H	301	NAP	O4D-C4D-C5D-O5D
2	B	301	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	O4D-C1D-N1N-C6N
2	C	301	NAP	O4D-C4D-C5D-O5D
2	F	301	NAP	O4D-C1D-N1N-C6N
2	K	301	NAP	C3D-C4D-C5D-O5D
2	K	301	NAP	O4D-C1D-N1N-C6N
2	A	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	C2B-O2B-P2B-O1X
2	F	301	NAP	C2B-O2B-P2B-O1X
2	K	301	NAP	C2B-O2B-P2B-O1X
2	L	301	NAP	C2B-O2B-P2B-O1X
2	N	301	NAP	C2B-O2B-P2B-O1X
2	O	301	NAP	C2B-O2B-P2B-O1X
2	P	301	NAP	C2B-O2B-P2B-O1X
2	L	301	NAP	O4D-C4D-C5D-O5D
2	O	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	C2B-O2B-P2B-O3X
2	E	301	NAP	C2B-O2B-P2B-O2X
2	F	301	NAP	C2B-O2B-P2B-O3X
2	L	301	NAP	C2B-O2B-P2B-O3X
2	N	301	NAP	C2B-O2B-P2B-O3X
2	M	301	NAP	O4B-C4B-C5B-O5B
2	P	301	NAP	C3D-C4D-C5D-O5D
2	C	301	NAP	C2B-O2B-P2B-O1X
2	G	301	NAP	C2B-O2B-P2B-O1X
2	H	301	NAP	C2B-O2B-P2B-O1X
2	I	301	NAP	C2B-O2B-P2B-O1X
2	J	301	NAP	C2B-O2B-P2B-O1X
2	M	301	NAP	C2B-O2B-P2B-O1X
2	A	301	NAP	PN-O3-PA-O2A
2	C	301	NAP	PN-O3-PA-O2A
2	M	301	NAP	PN-O3-PA-O2A
2	P	301	NAP	PN-O3-PA-O2A
2	C	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	J	301	NAP	O4B-C4B-C5B-O5B

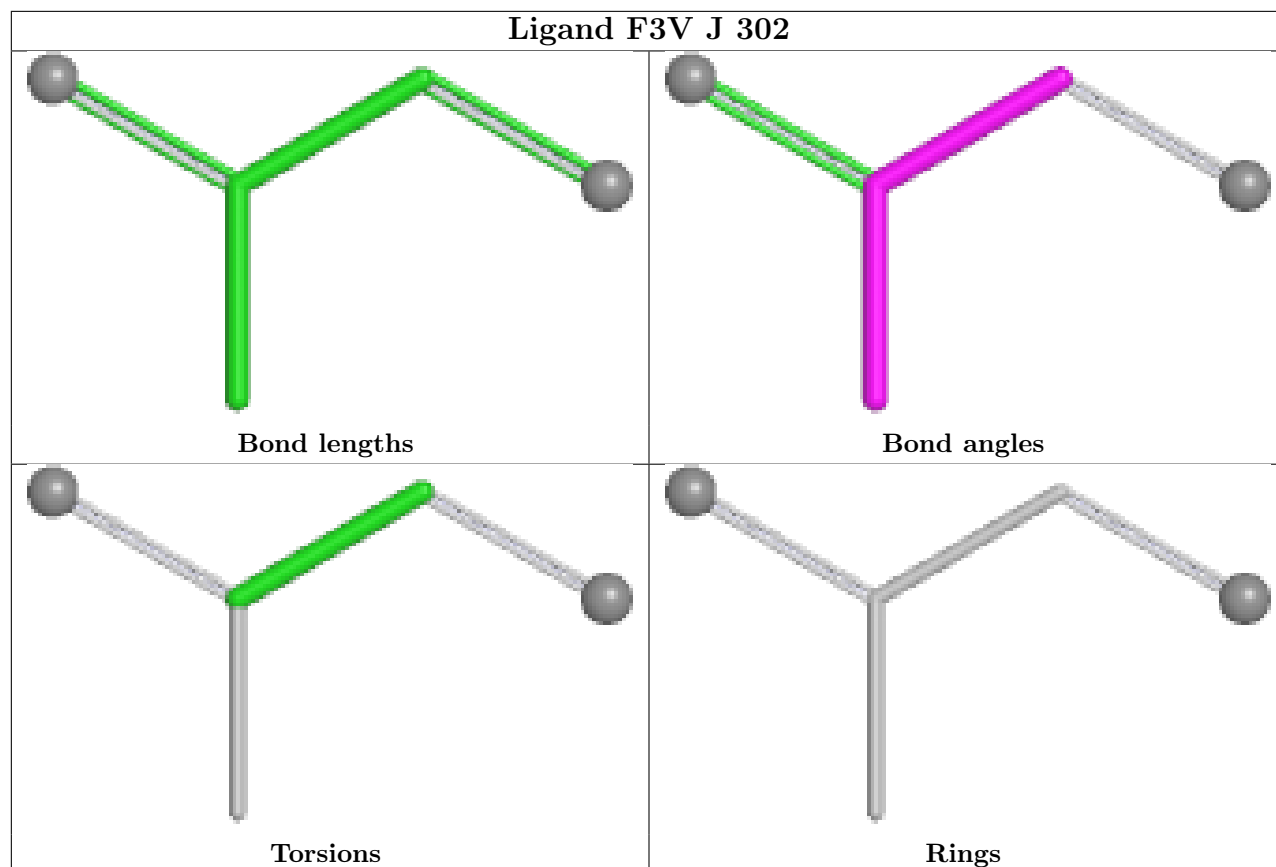
There are no ring outliers.

16 monomers are involved in 35 short contacts:

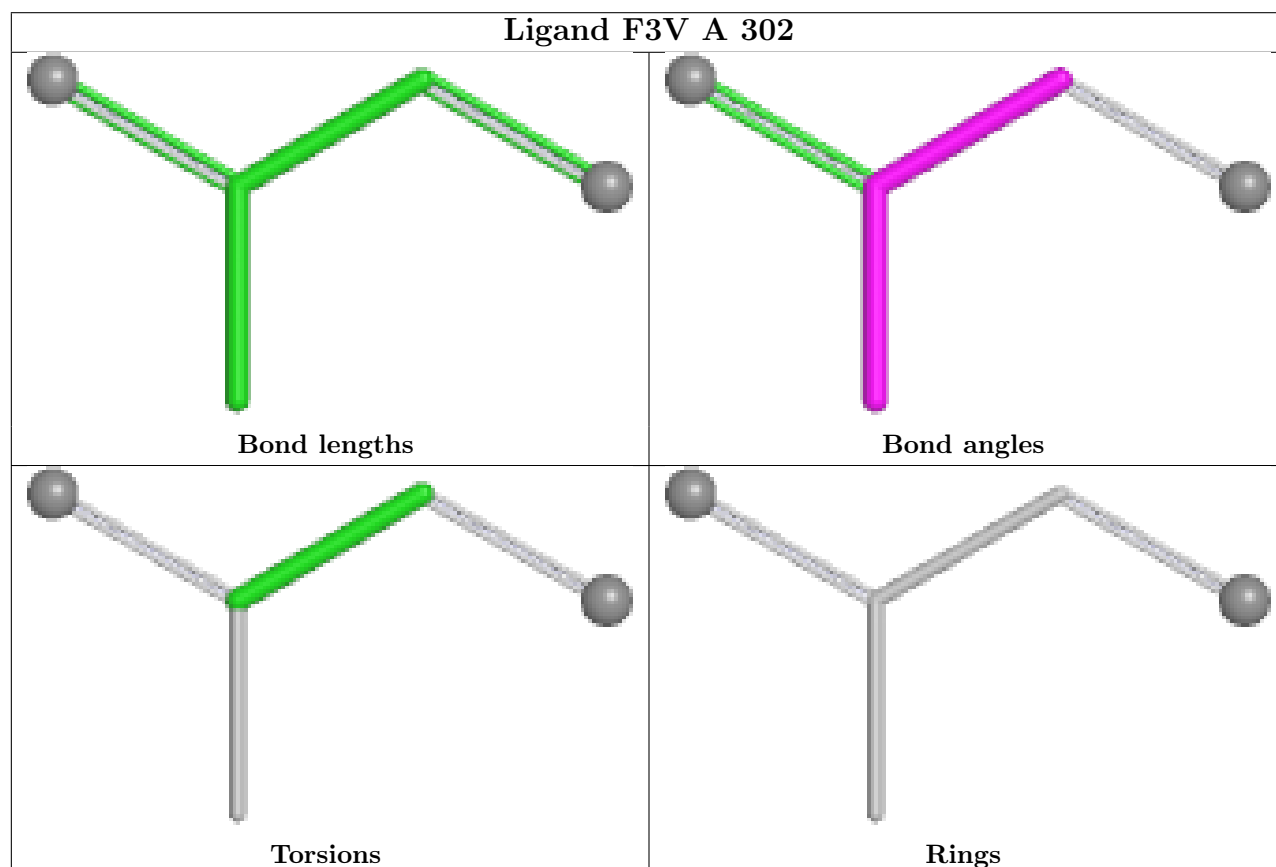
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	2	0
2	J	301	NAP	1	0
2	N	301	NAP	5	0
2	L	301	NAP	2	0
2	B	301	NAP	3	0
2	E	301	NAP	2	0
2	D	301	NAP	2	0
2	G	301	NAP	2	0
2	F	301	NAP	2	0
2	O	301	NAP	3	0
2	P	301	NAP	2	0
2	K	301	NAP	2	0
2	C	301	NAP	1	0
2	M	301	NAP	2	0
2	I	301	NAP	3	0
2	H	301	NAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

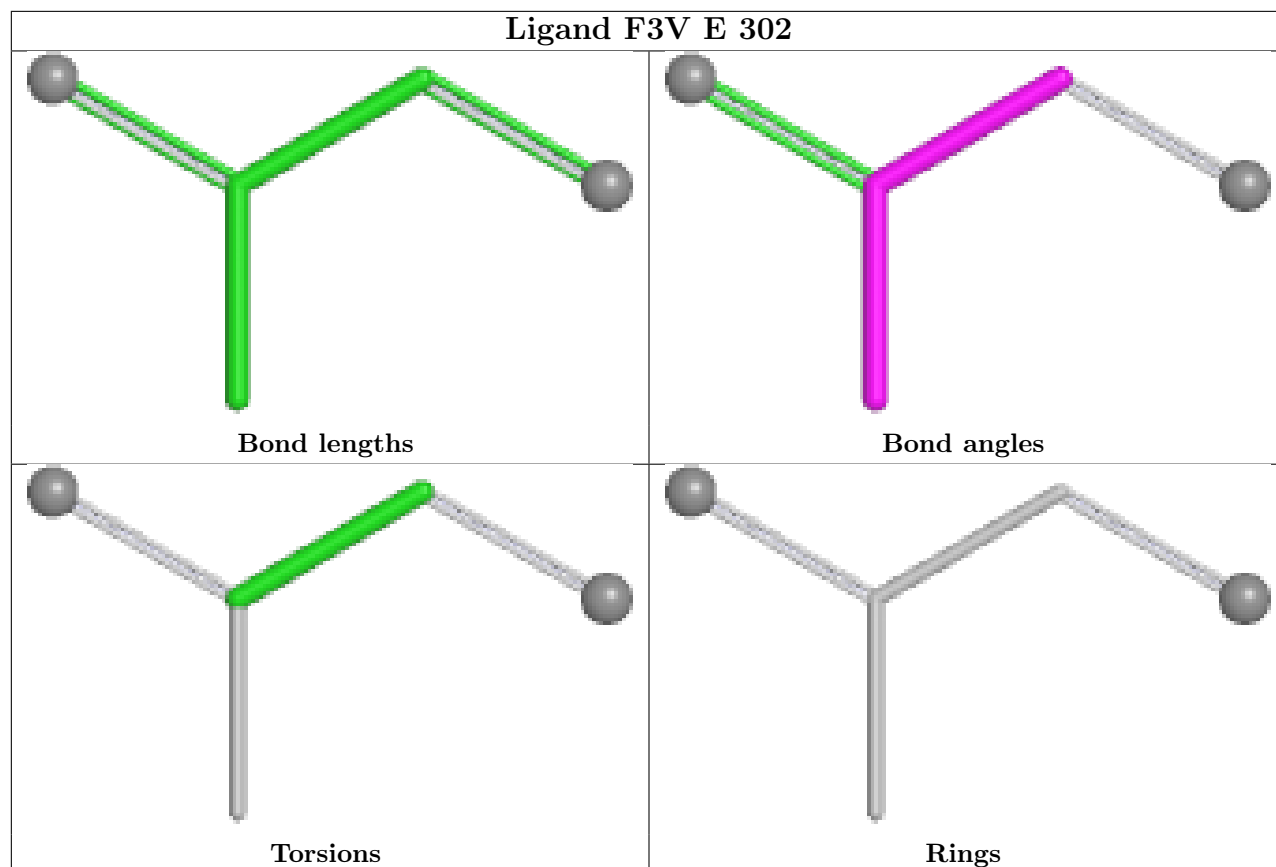
Ligand F3V J 302



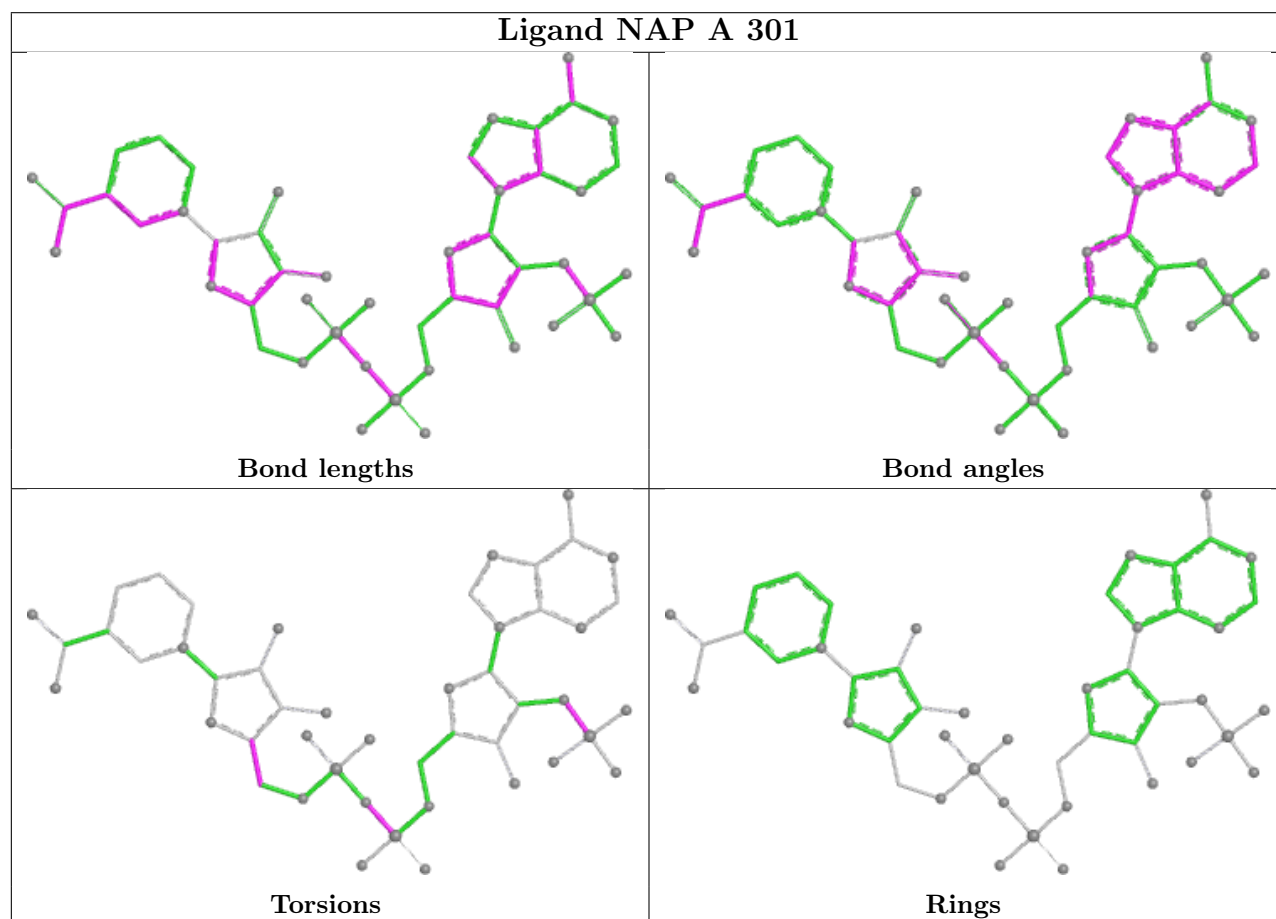
Ligand F3V A 302

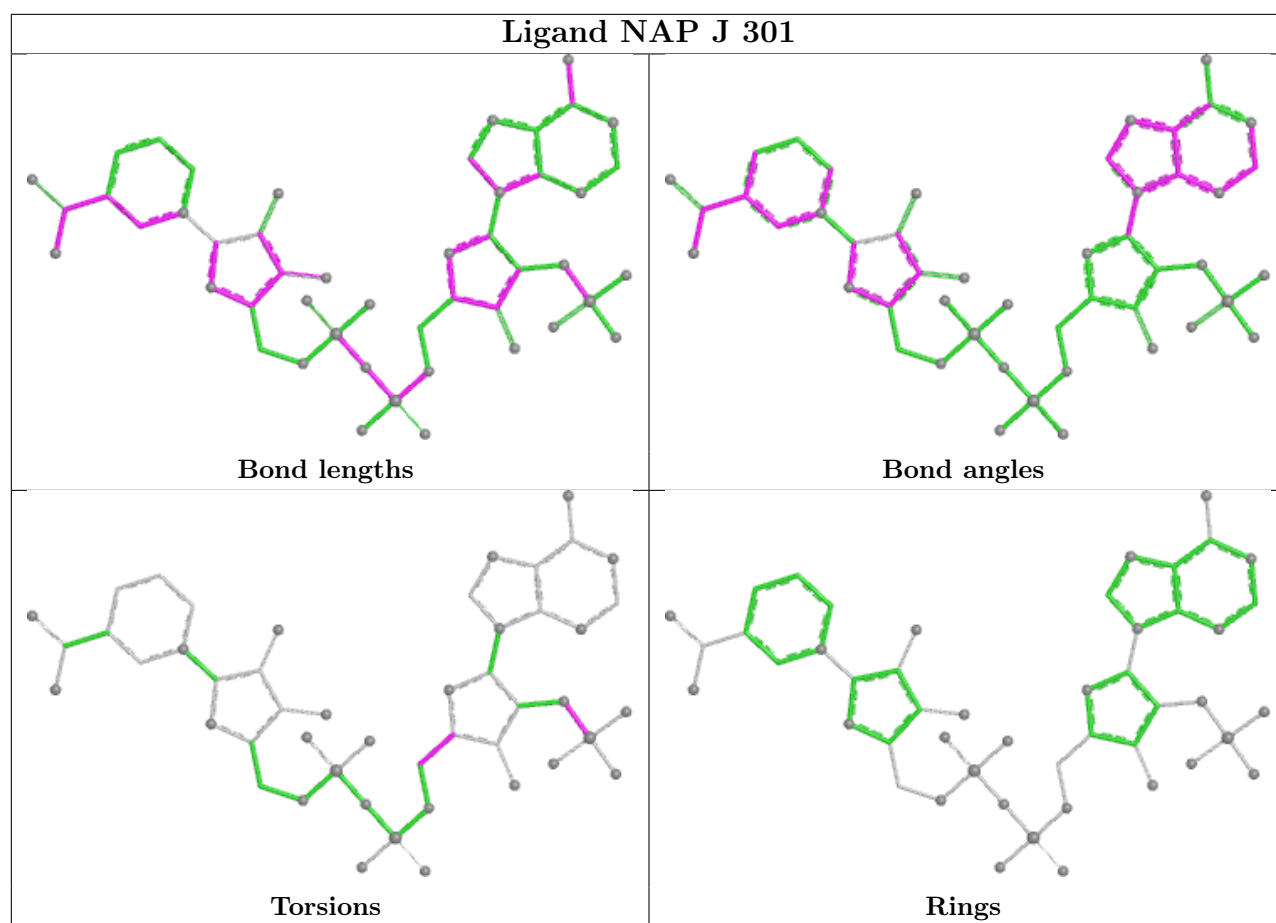


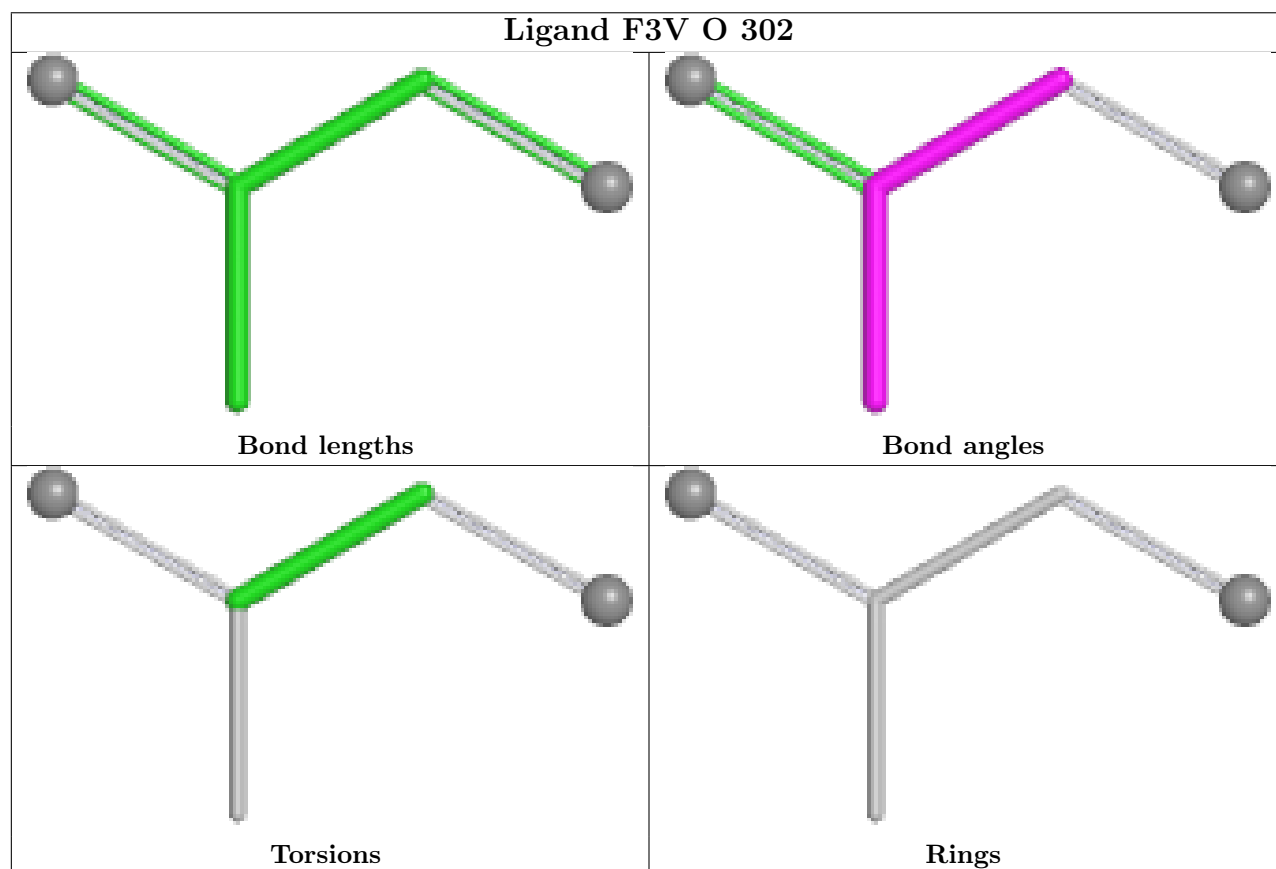
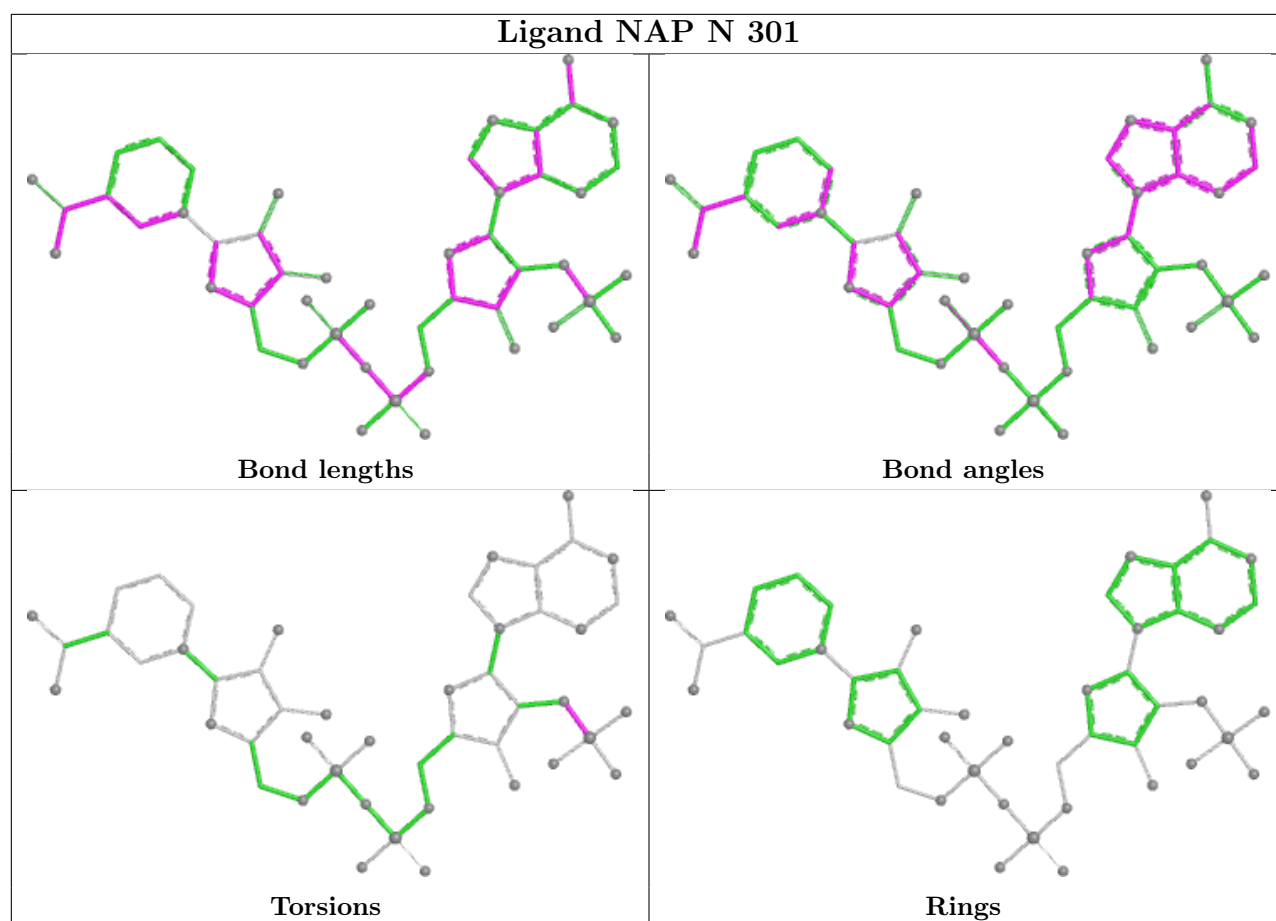
Ligand F3V E 302



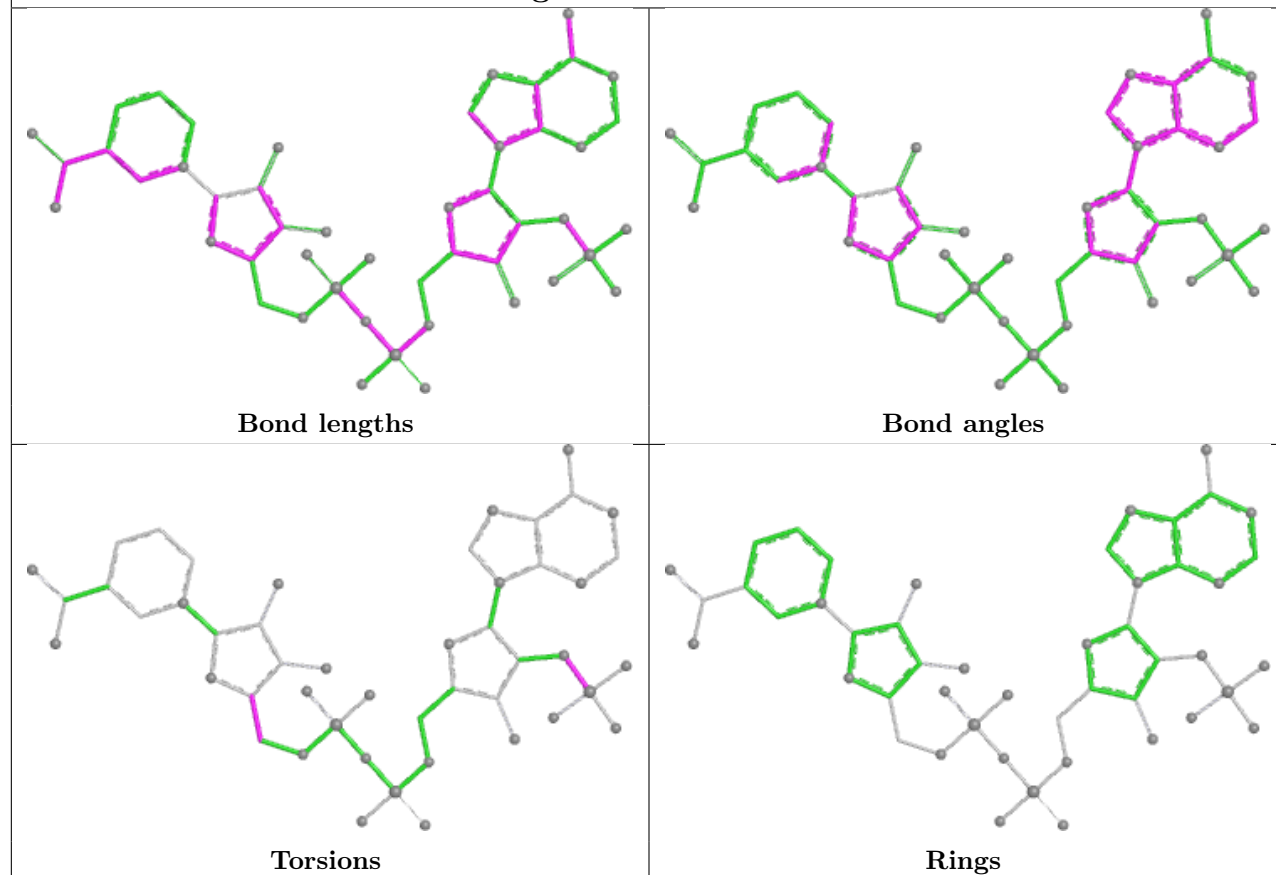
Ligand NAP A 301



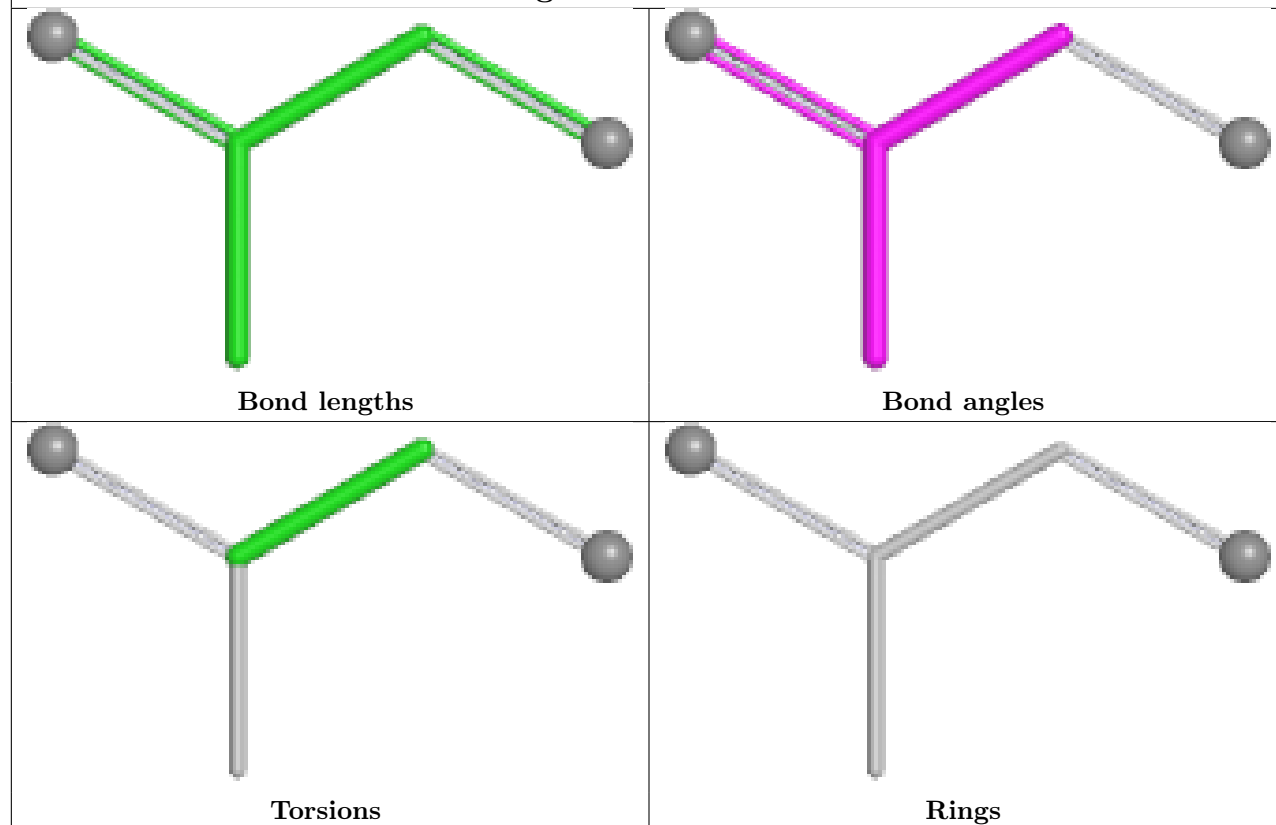




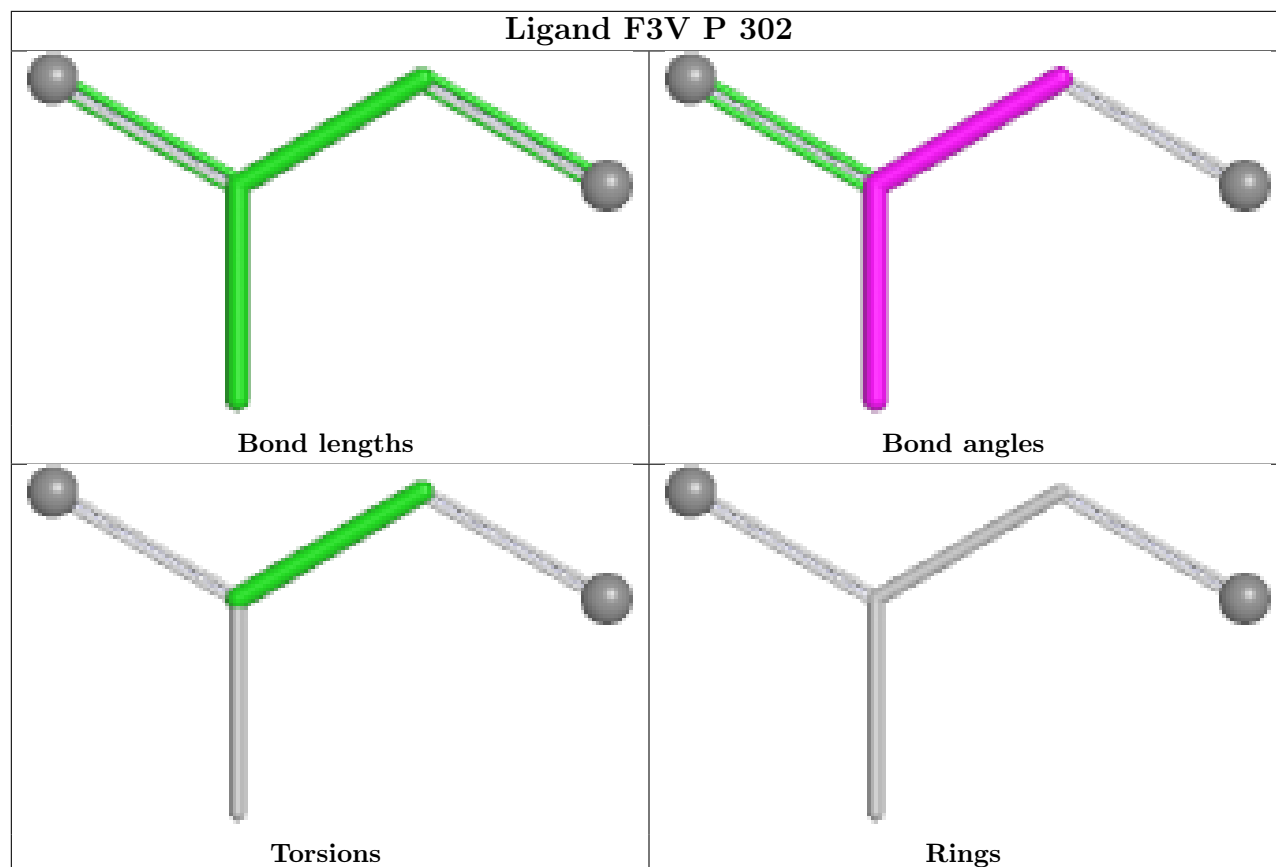
Ligand NAP L 301



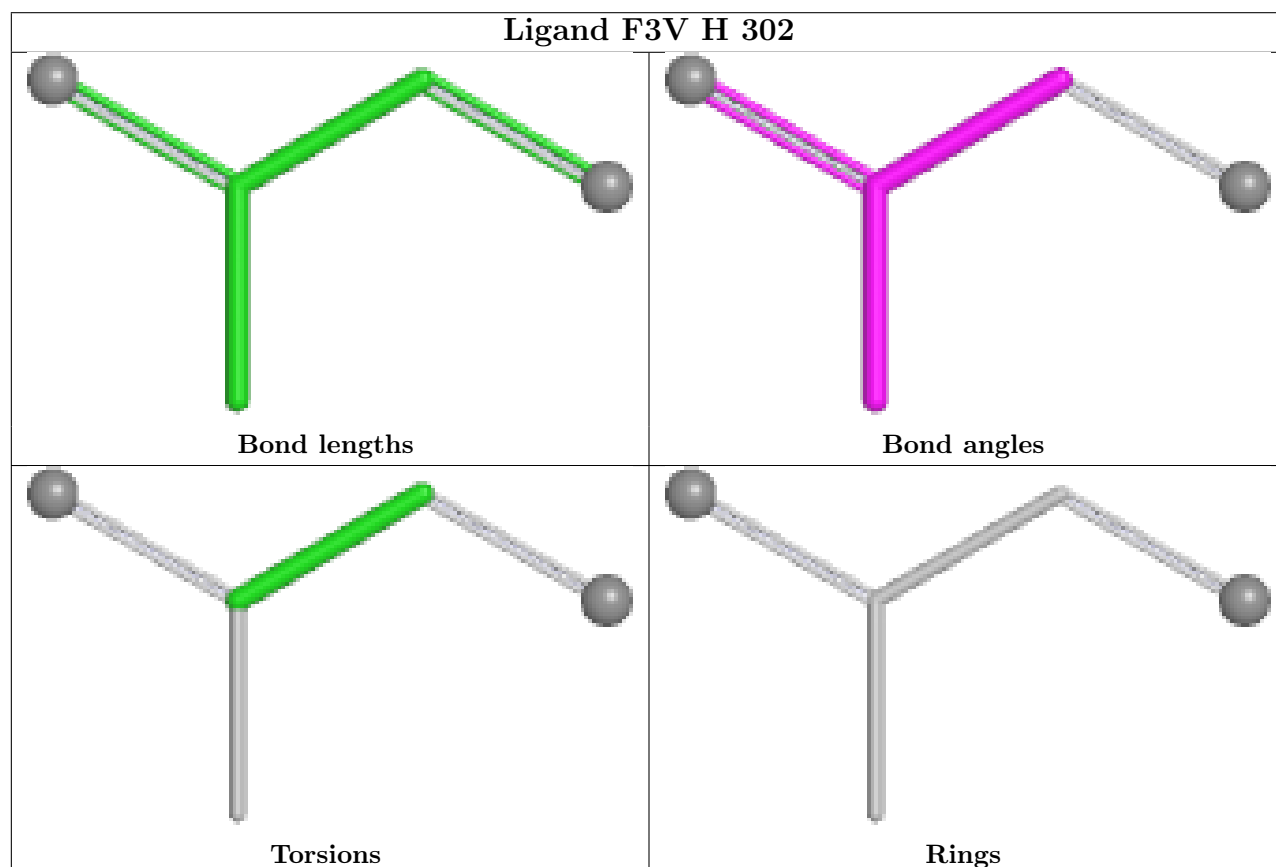
Ligand F3V B 302

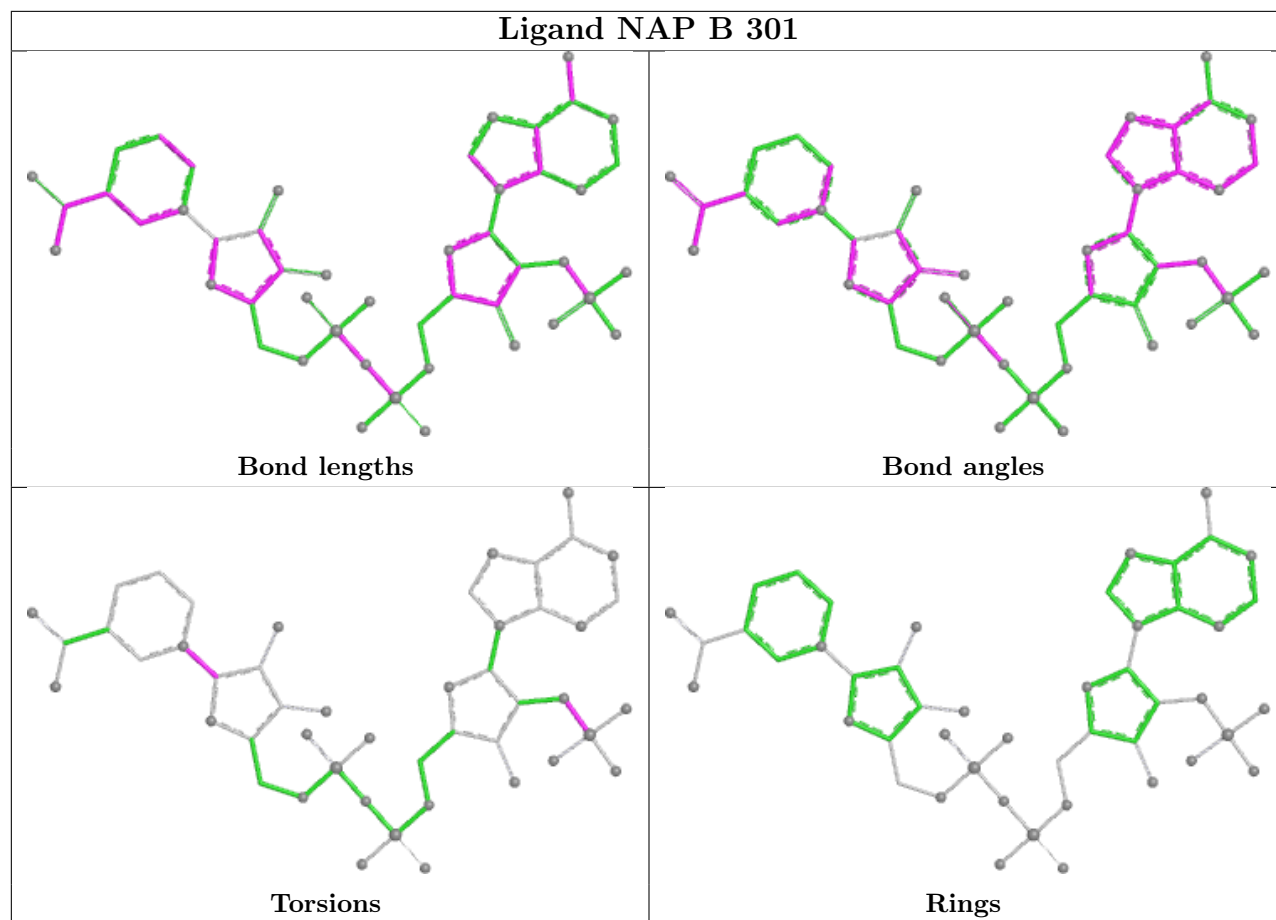


Ligand F3V P 302

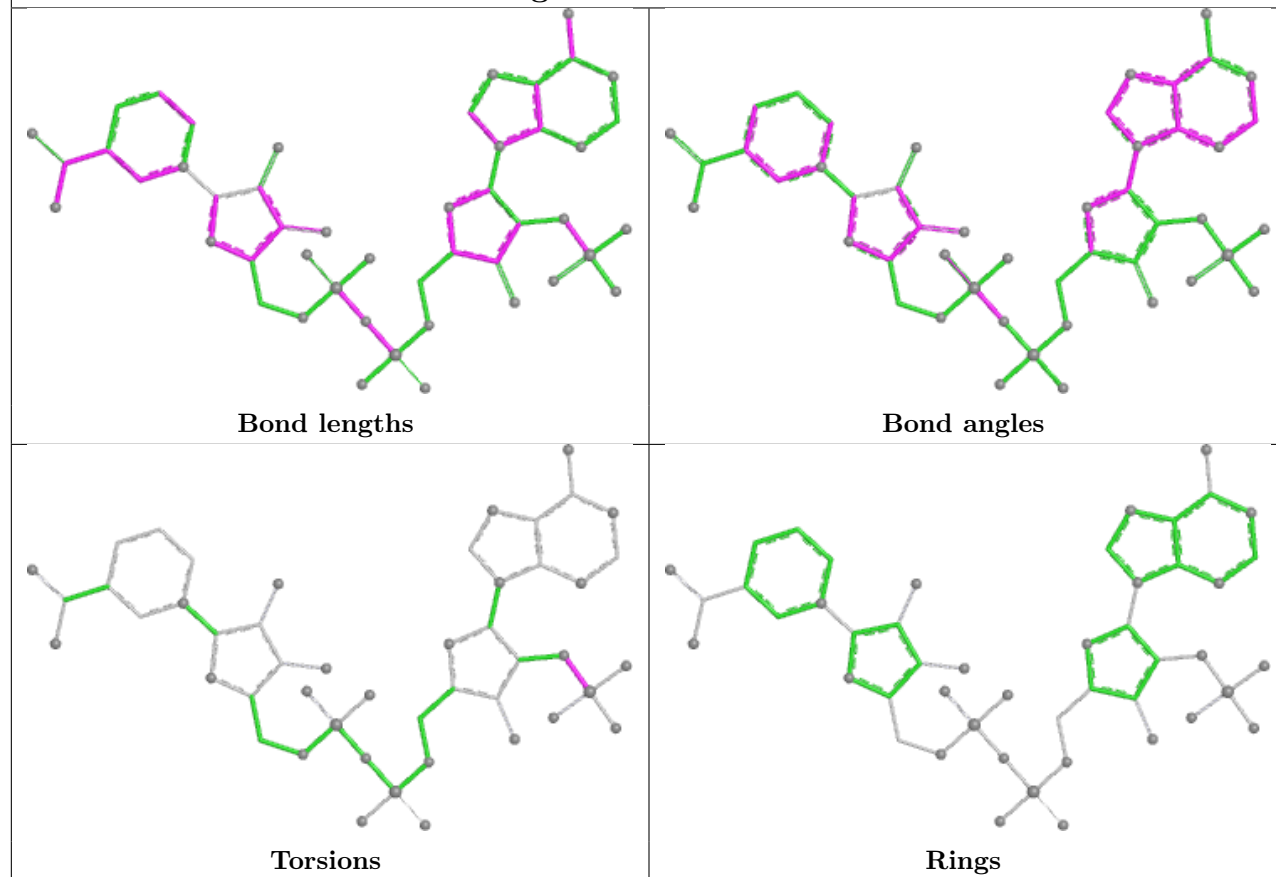


Ligand F3V H 302

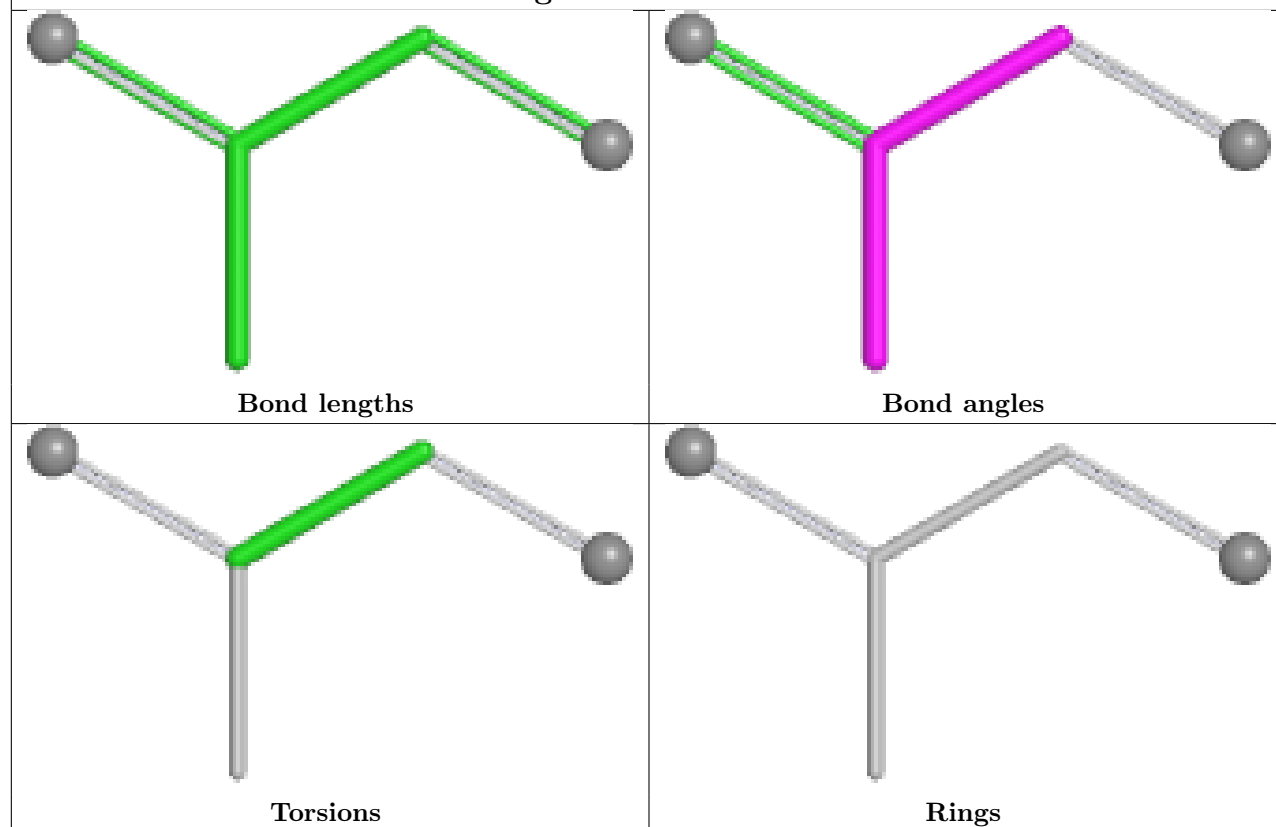




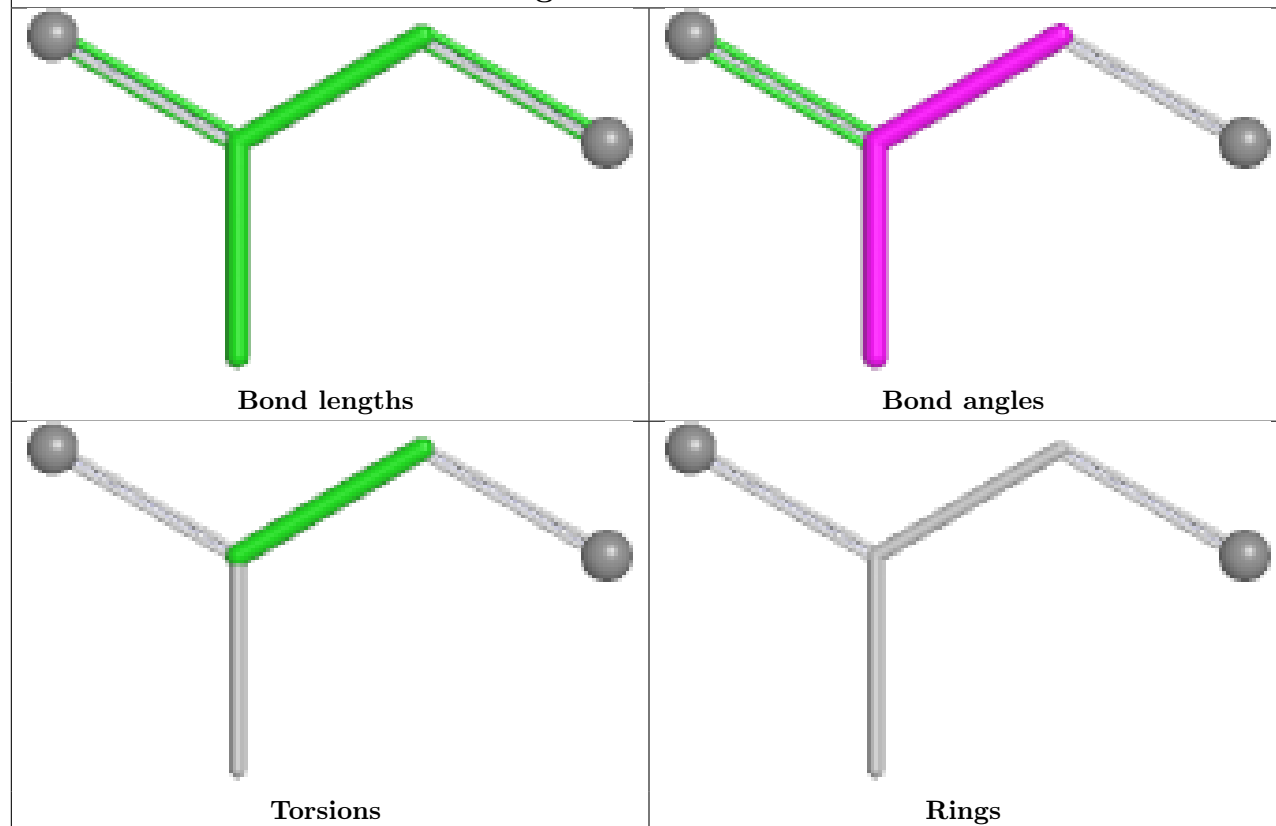
Ligand NAP E 301



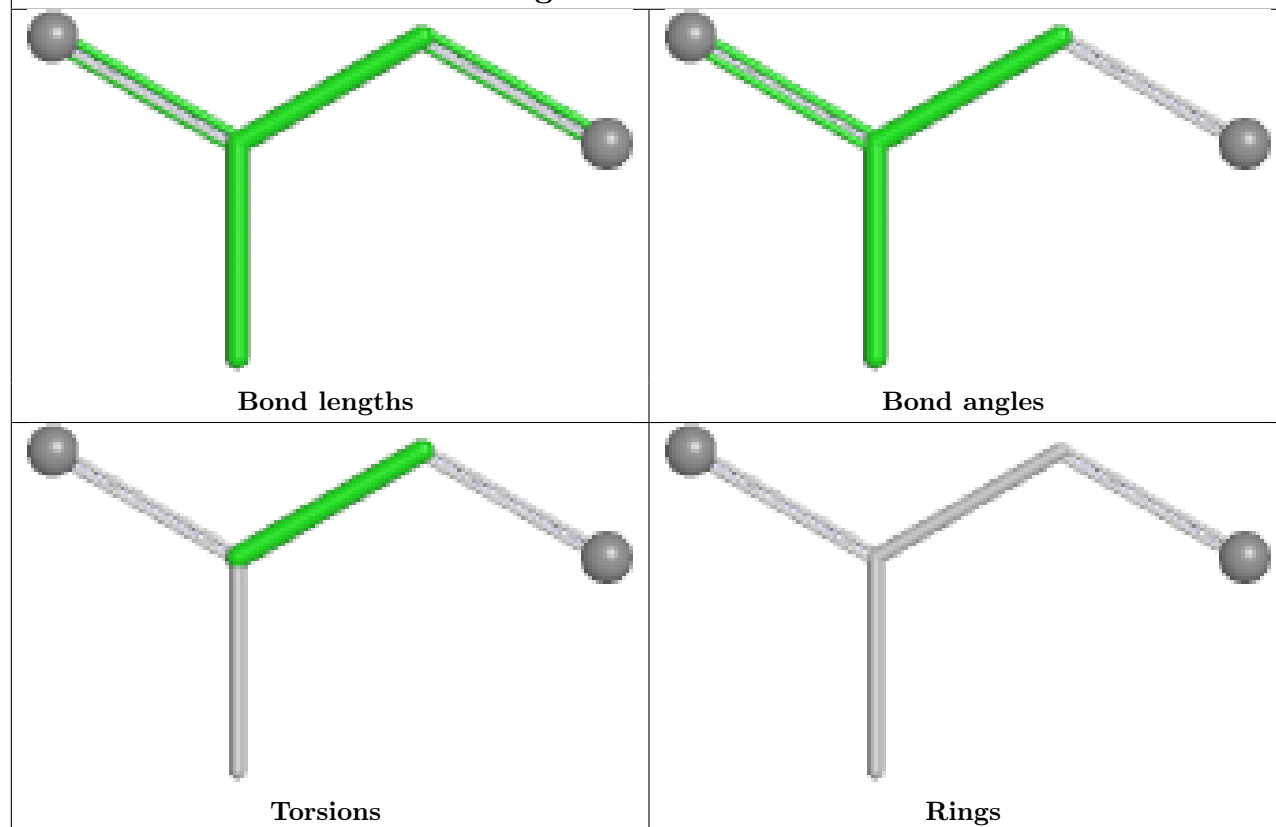
Ligand F3V K 302



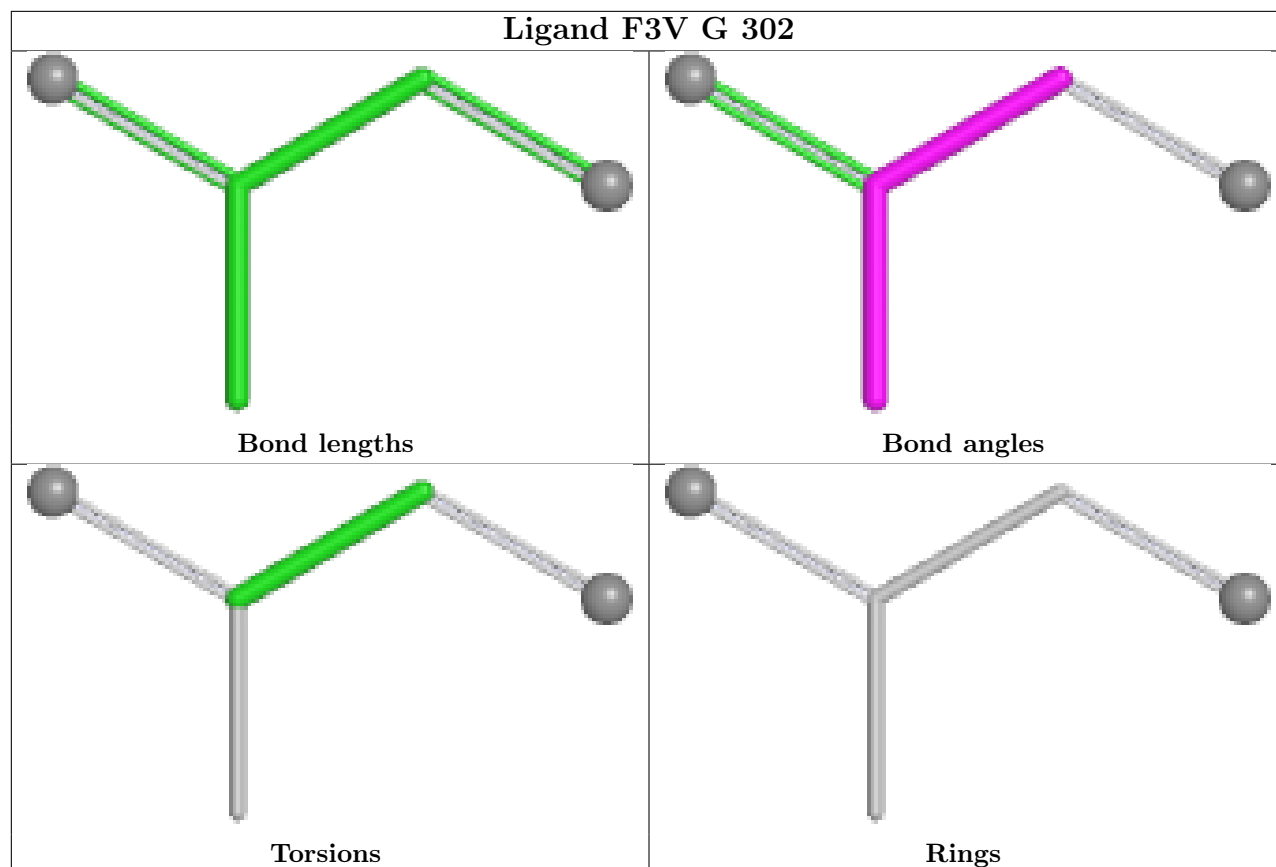
Ligand F3V C 302



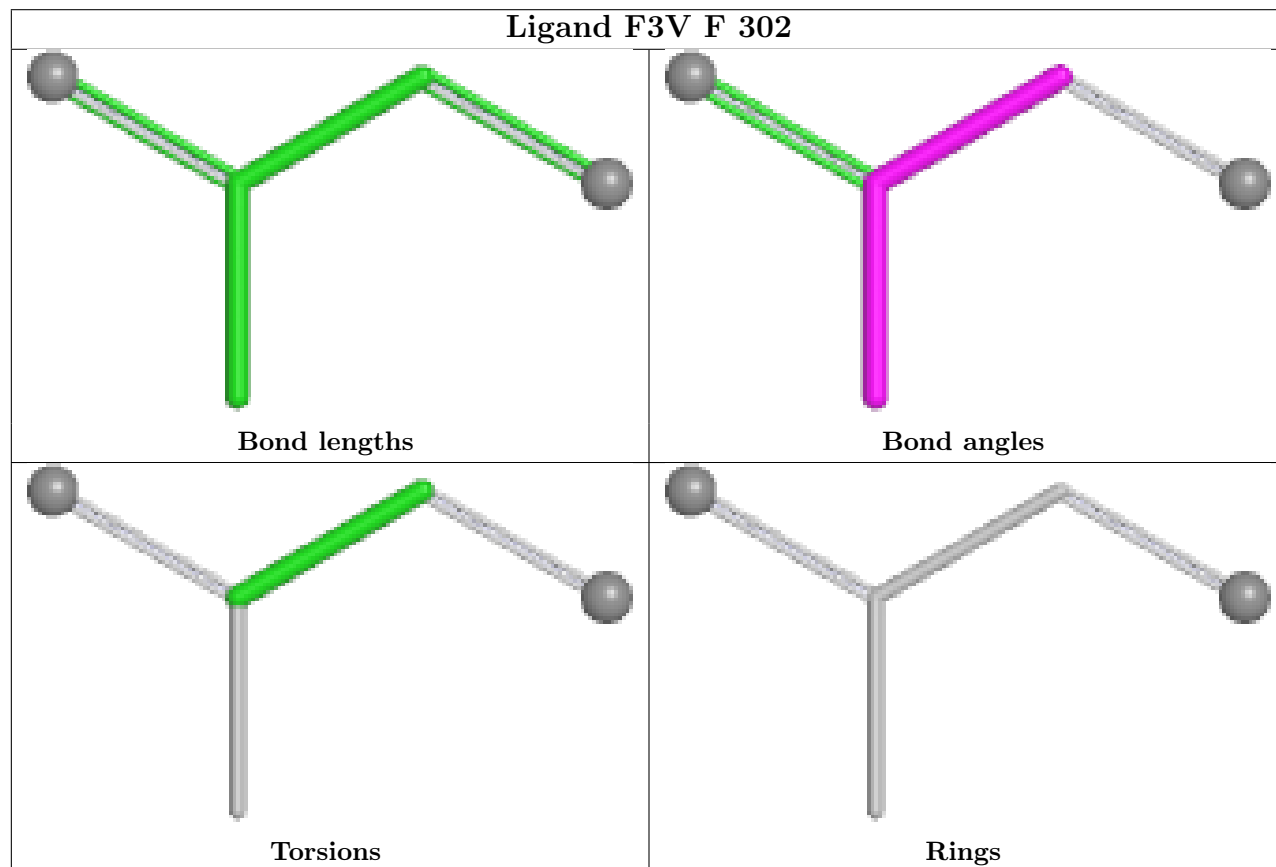
Ligand F3V D 302



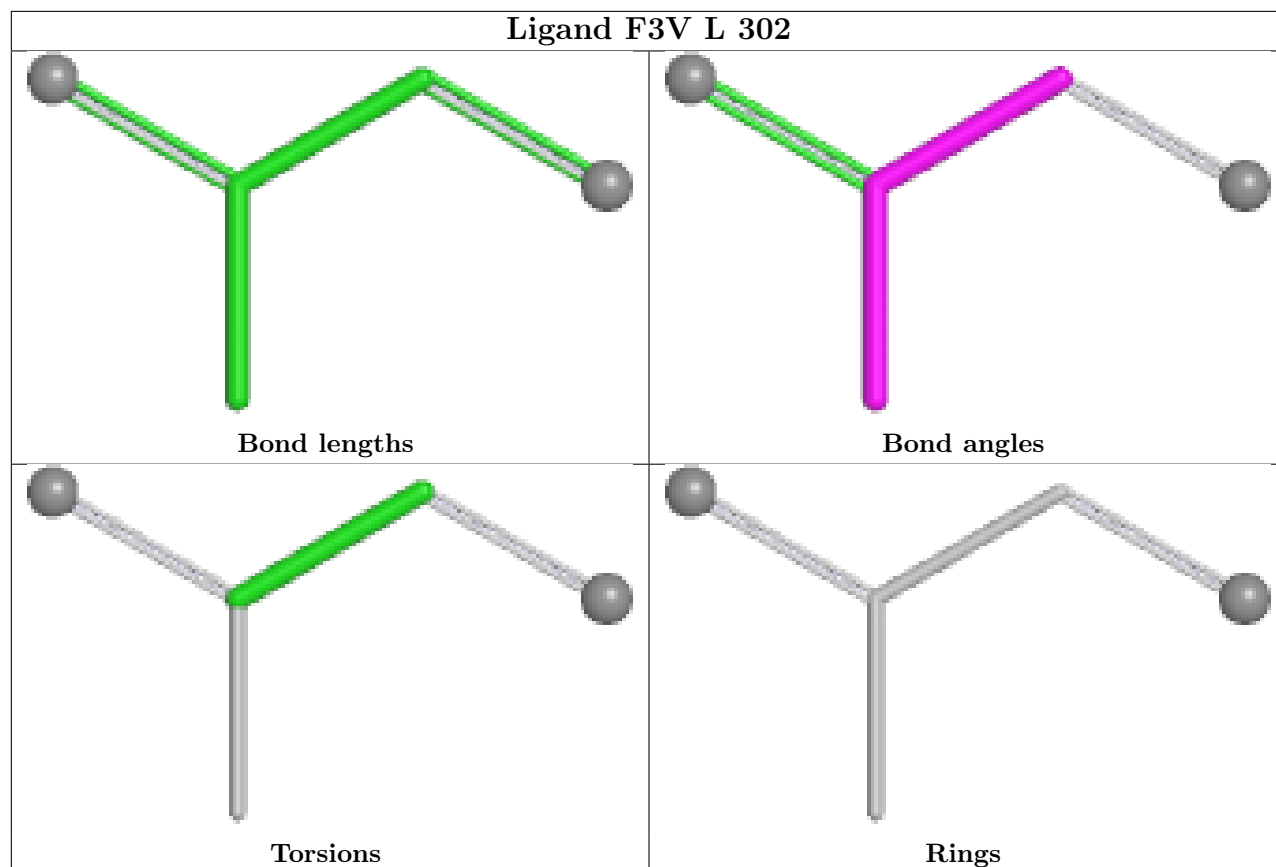
Ligand F3V G 302



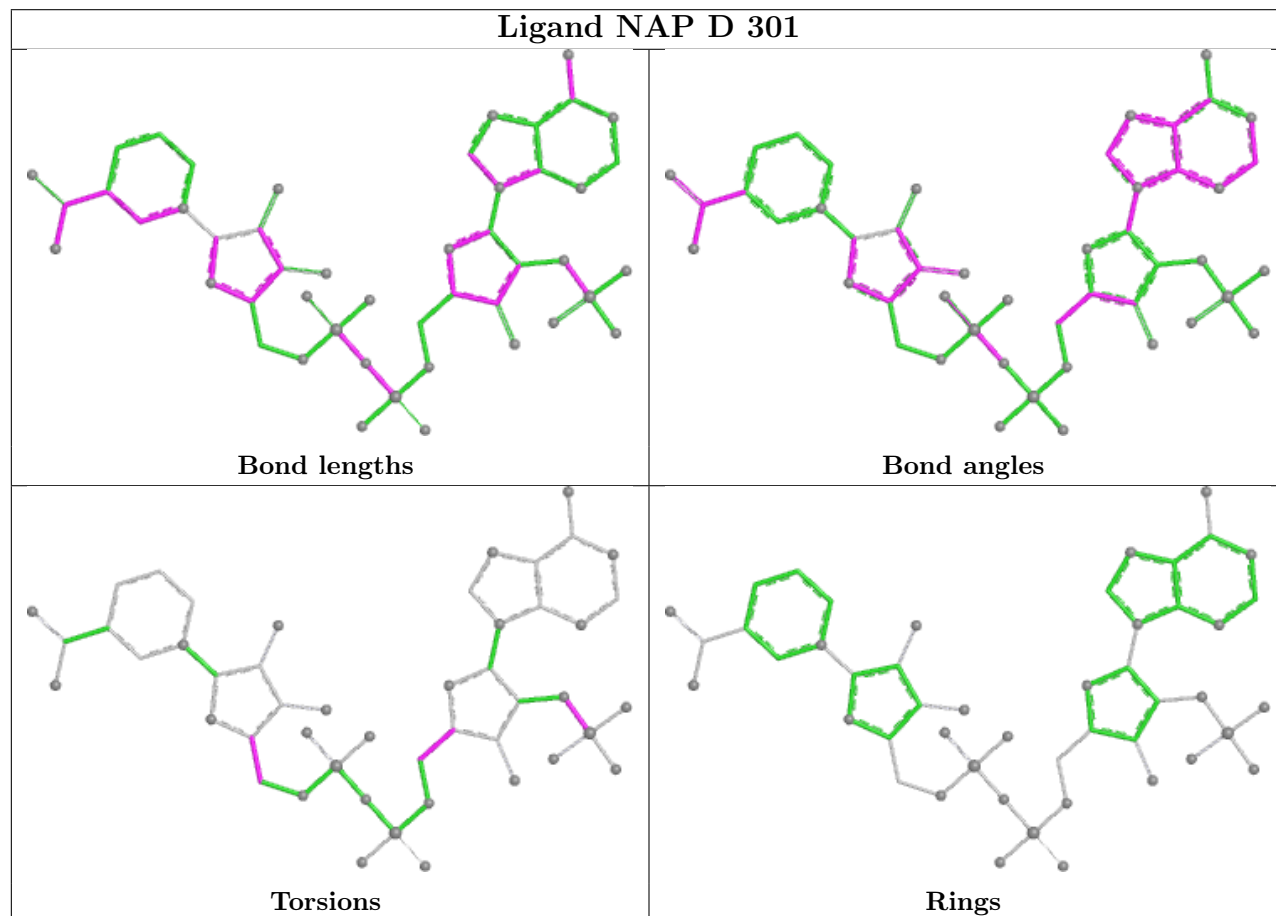
Ligand F3V F 302

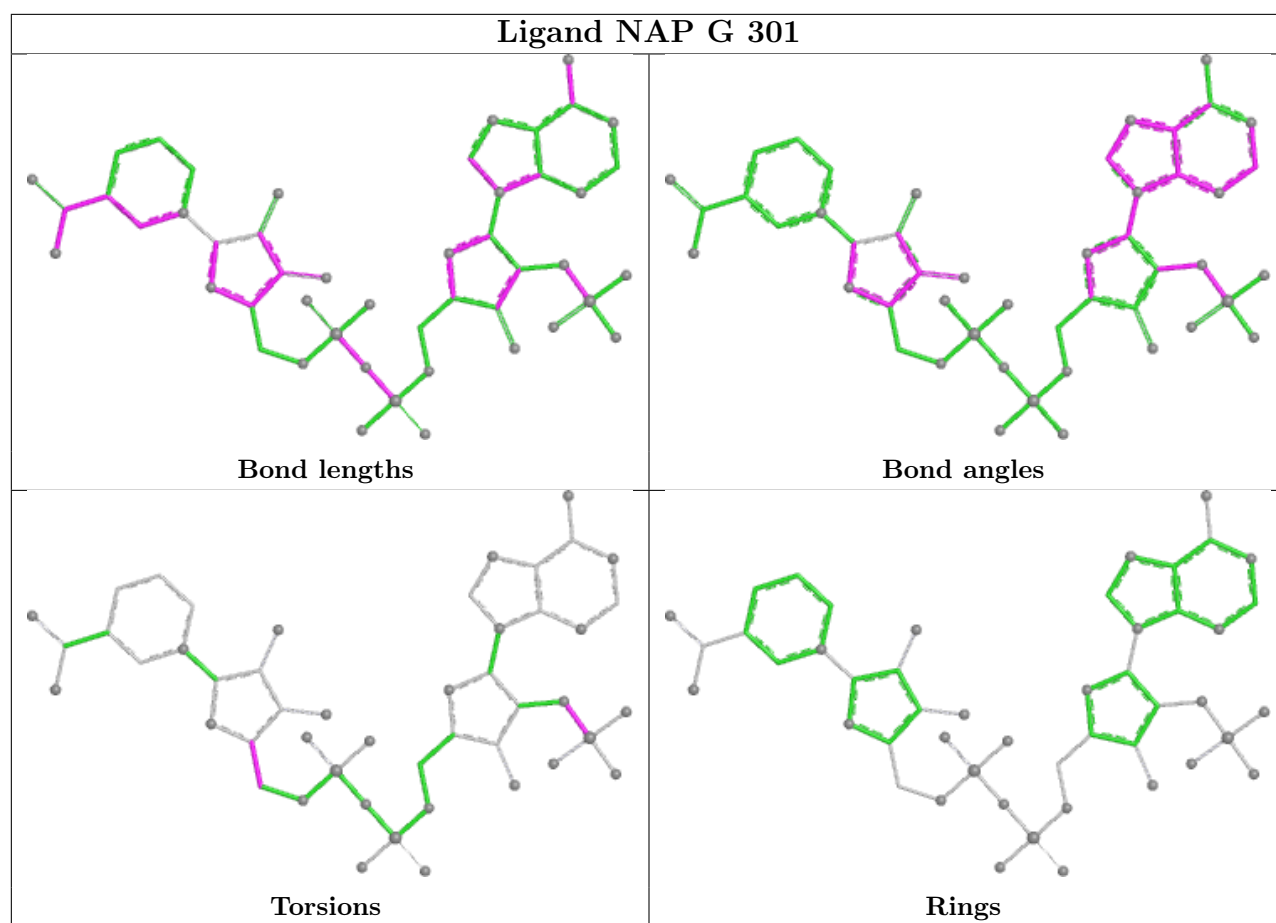


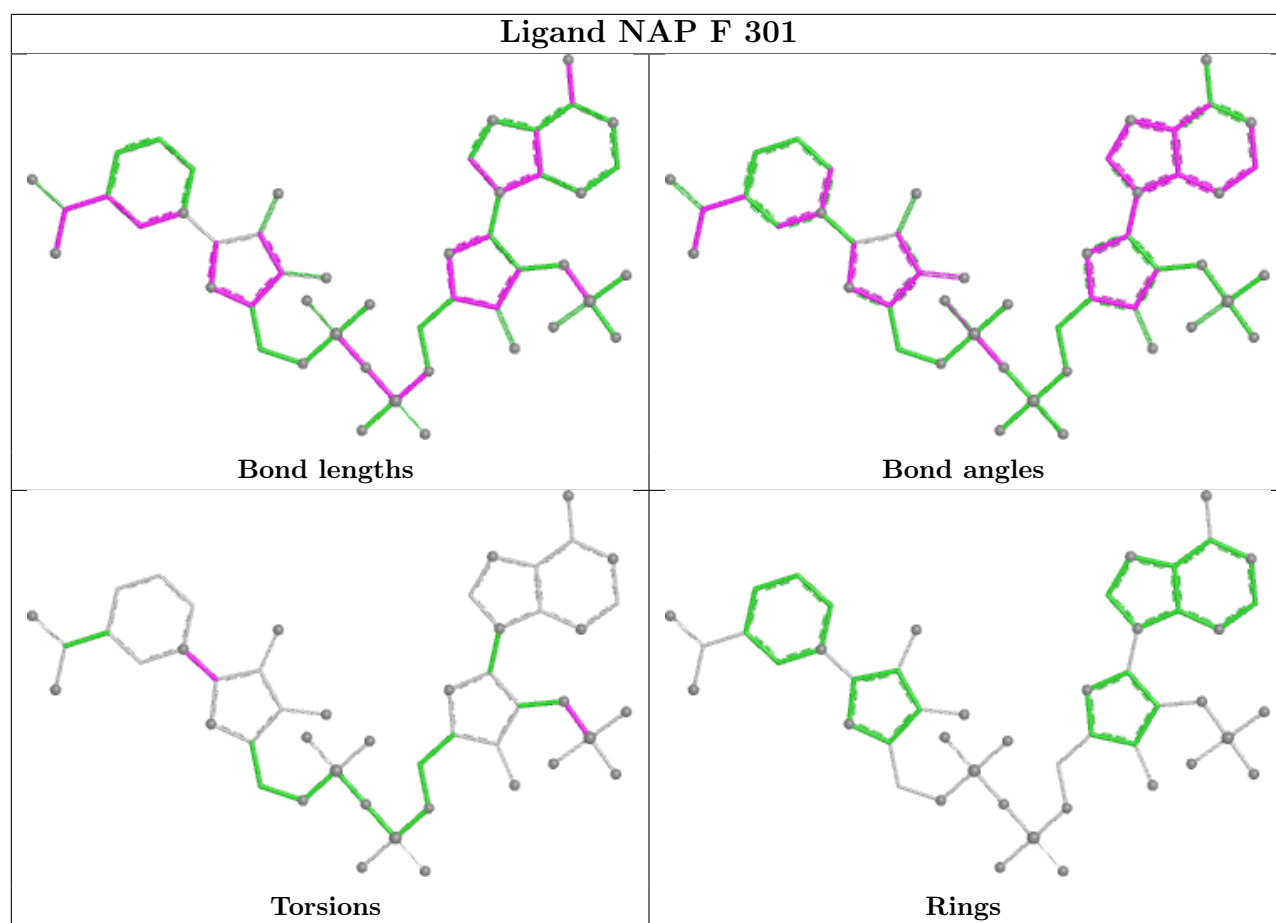
Ligand F3V L 302

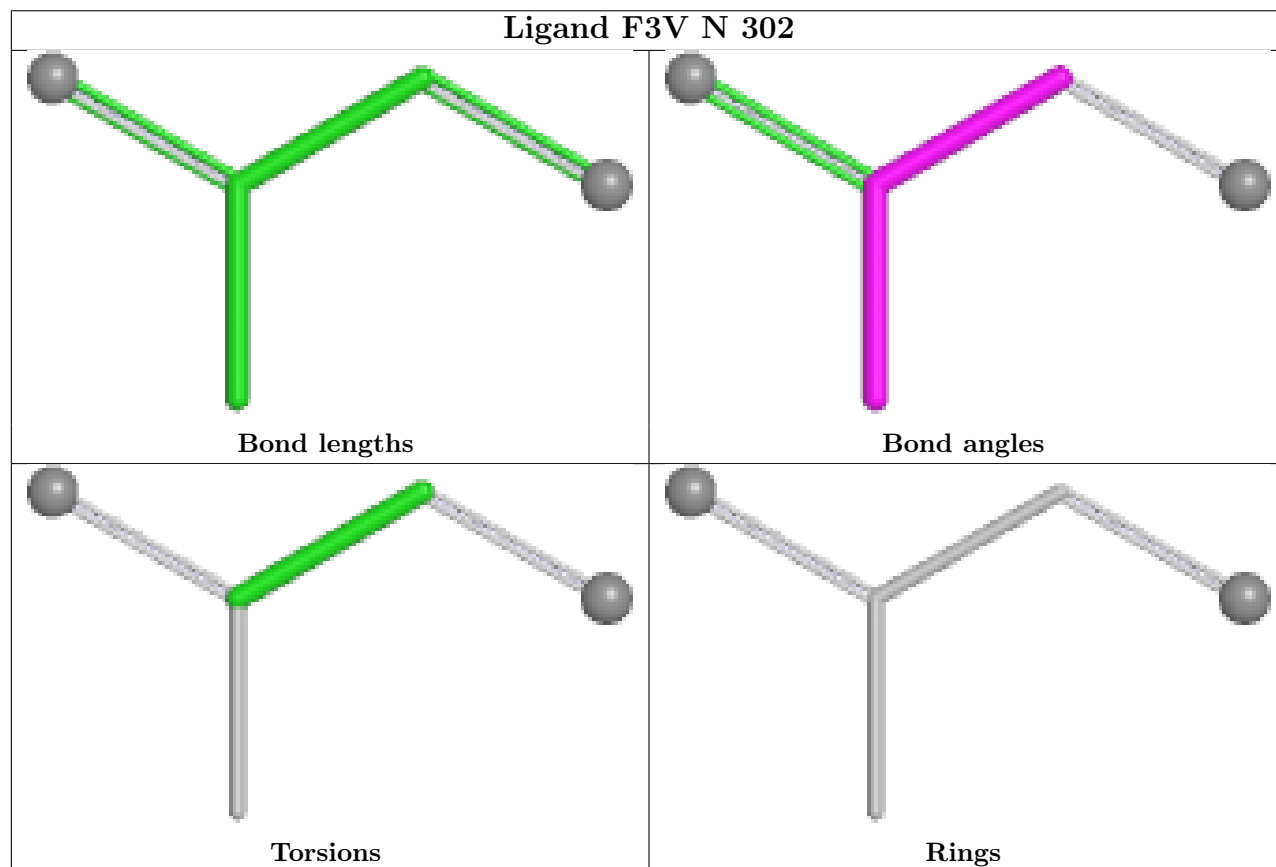
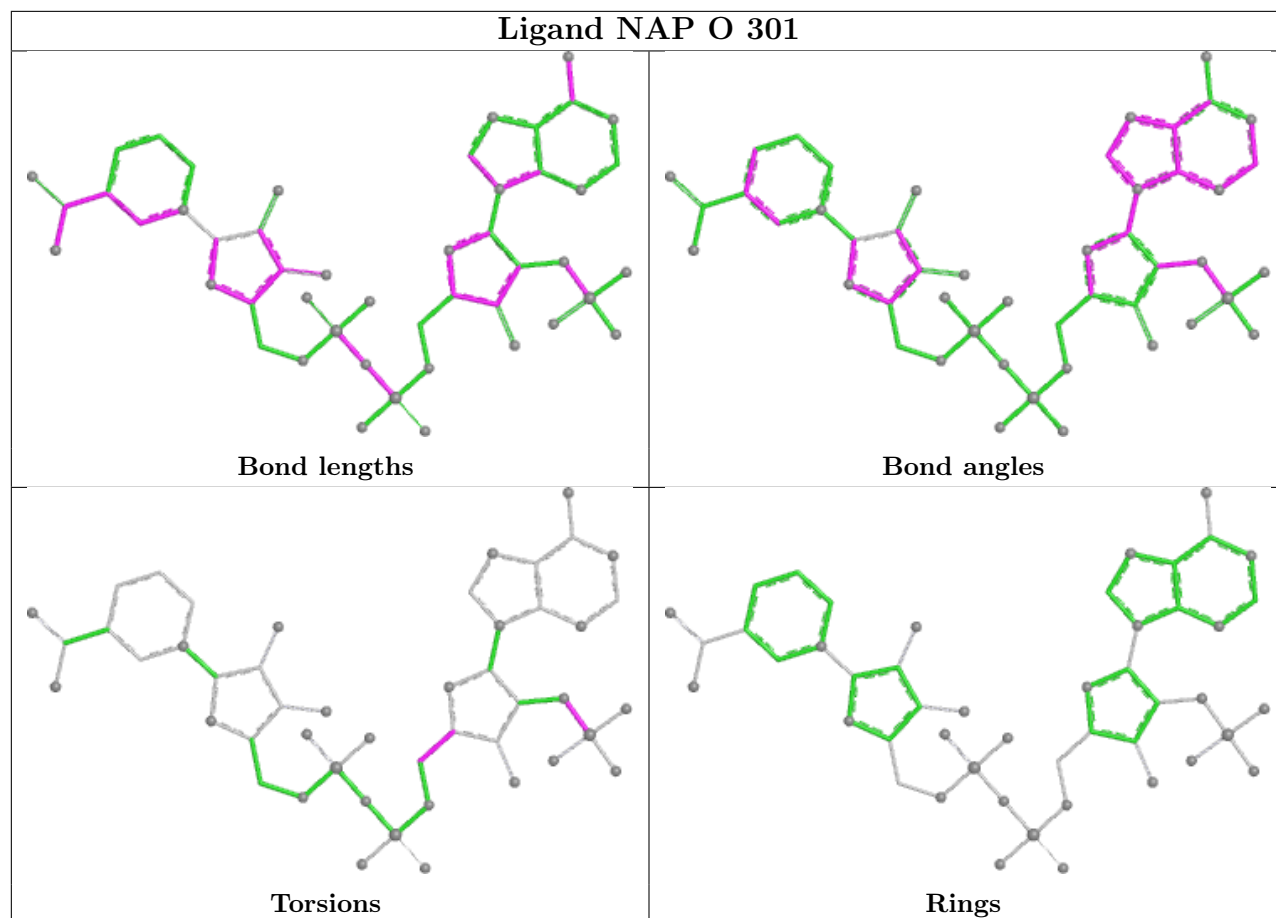


Ligand NAP D 301

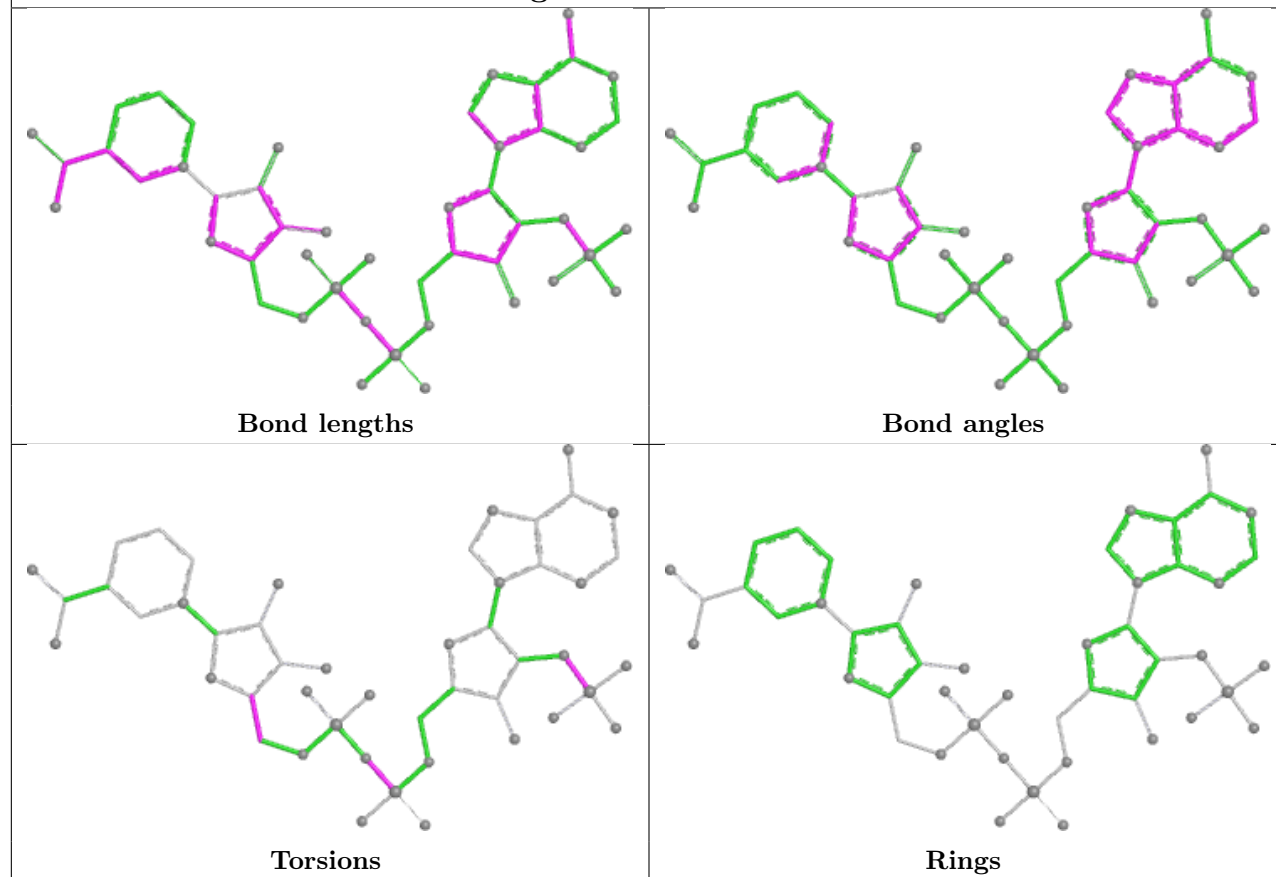




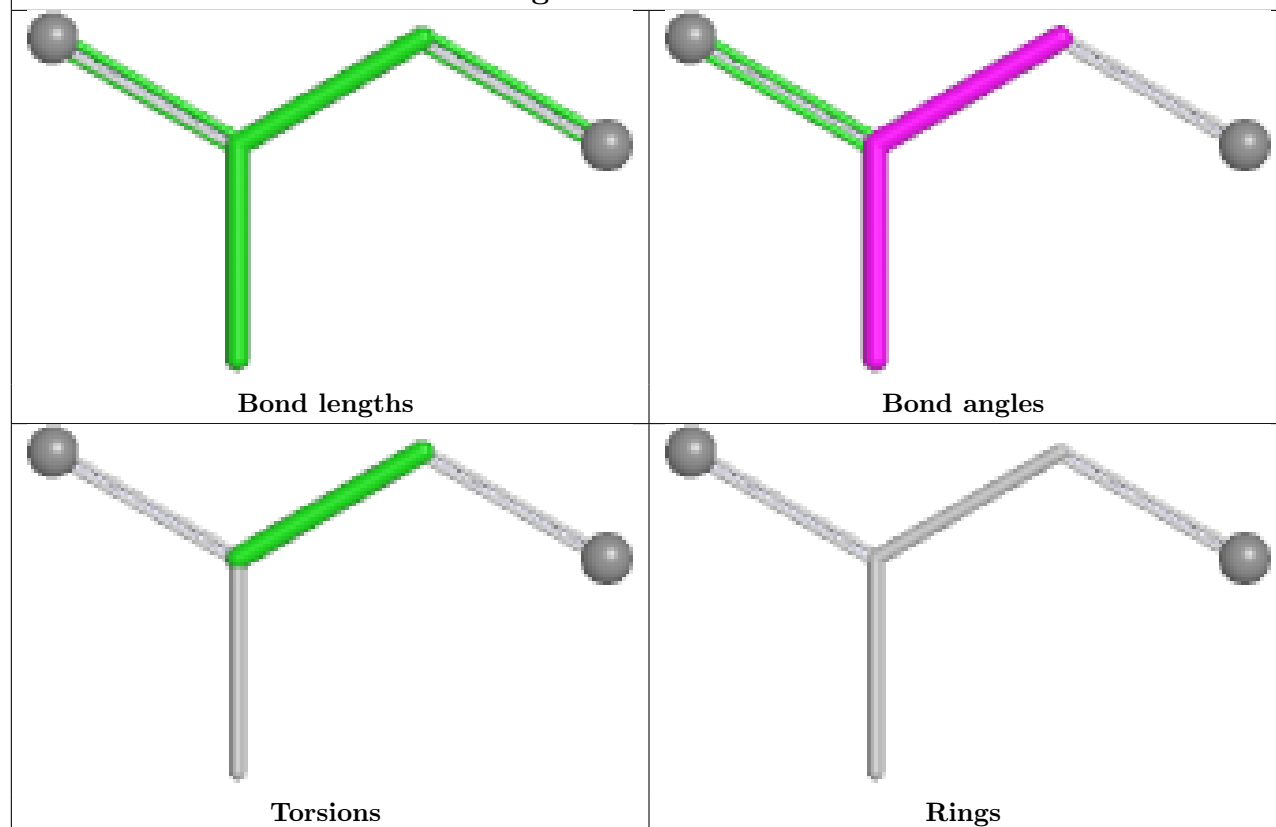


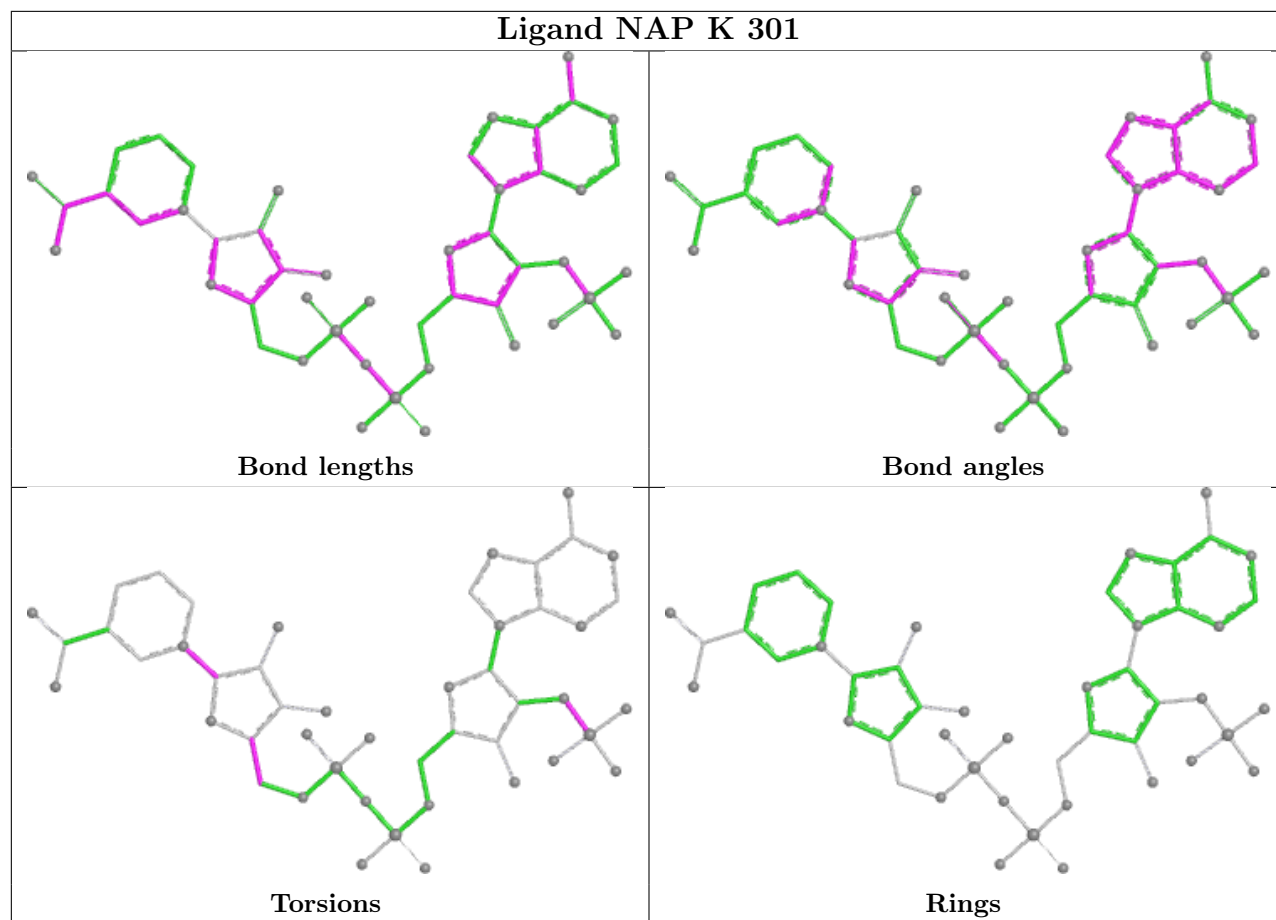


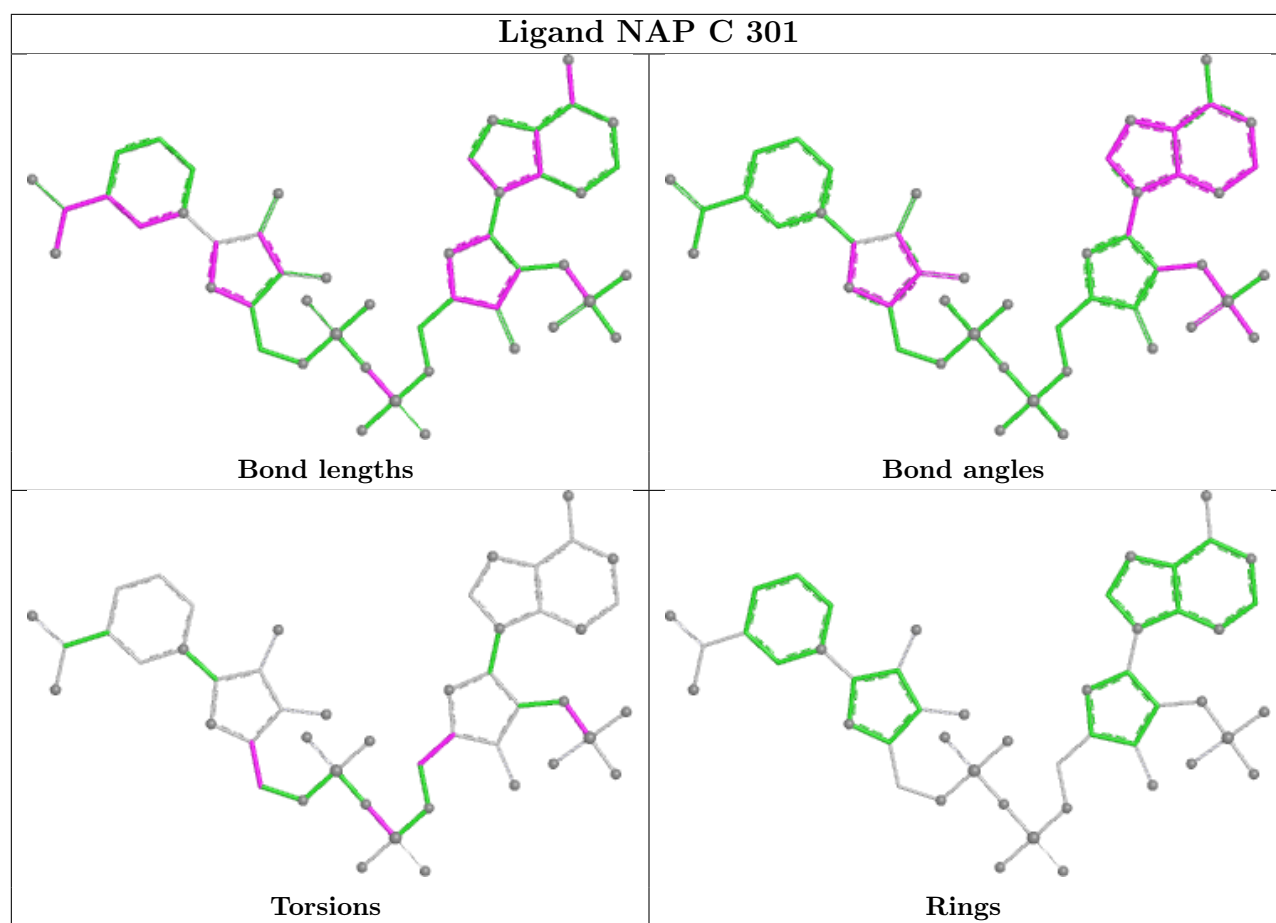
Ligand NAP P 301

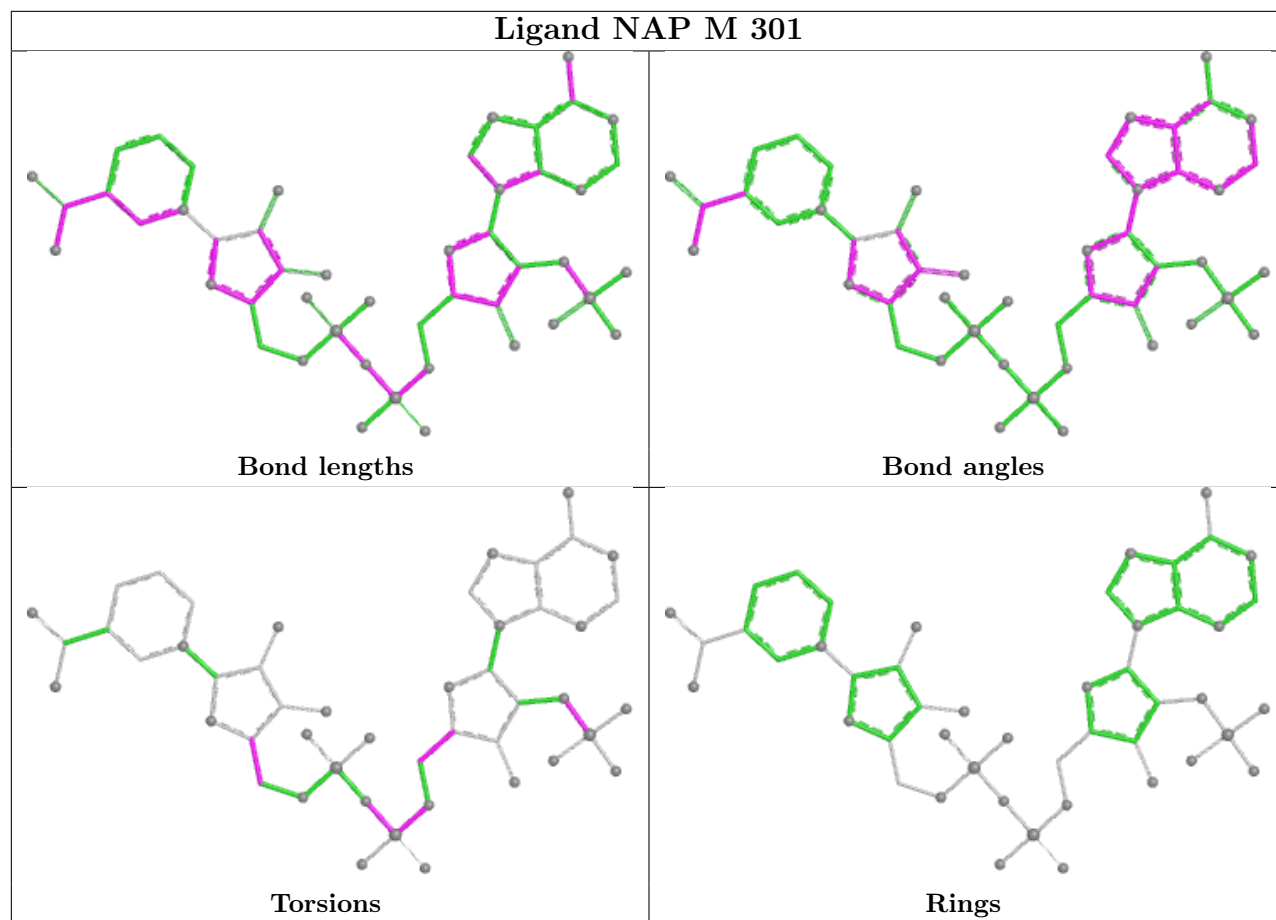


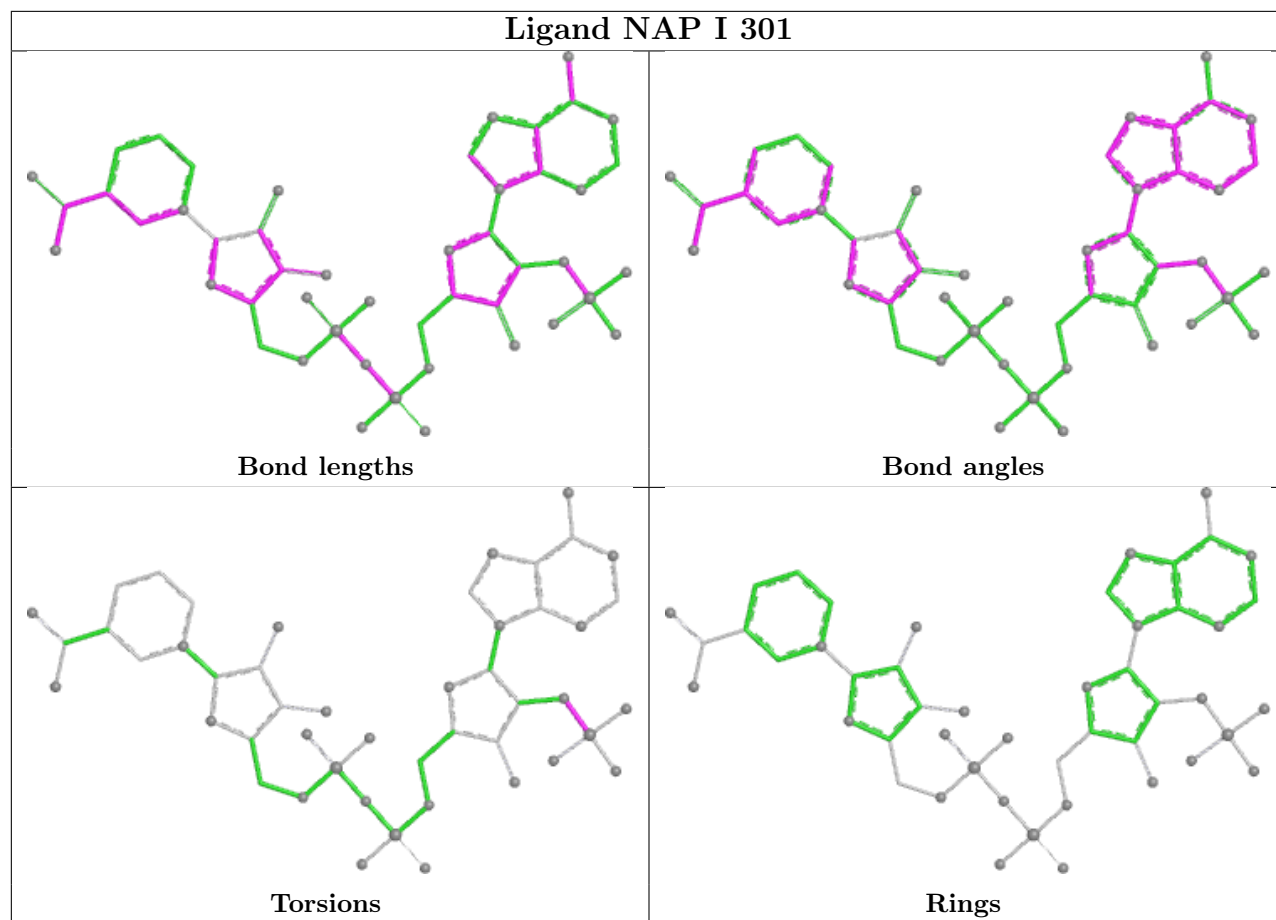
Ligand F3V M 302

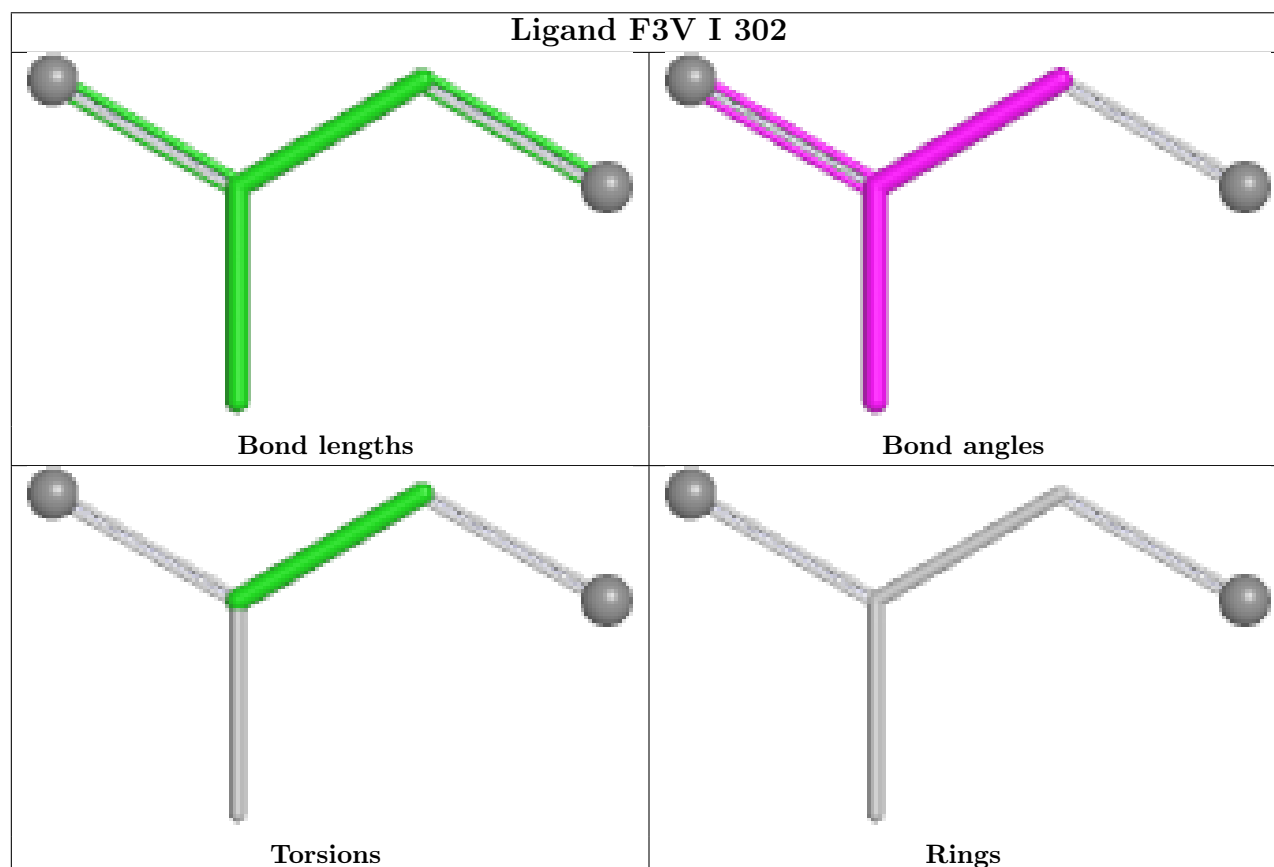
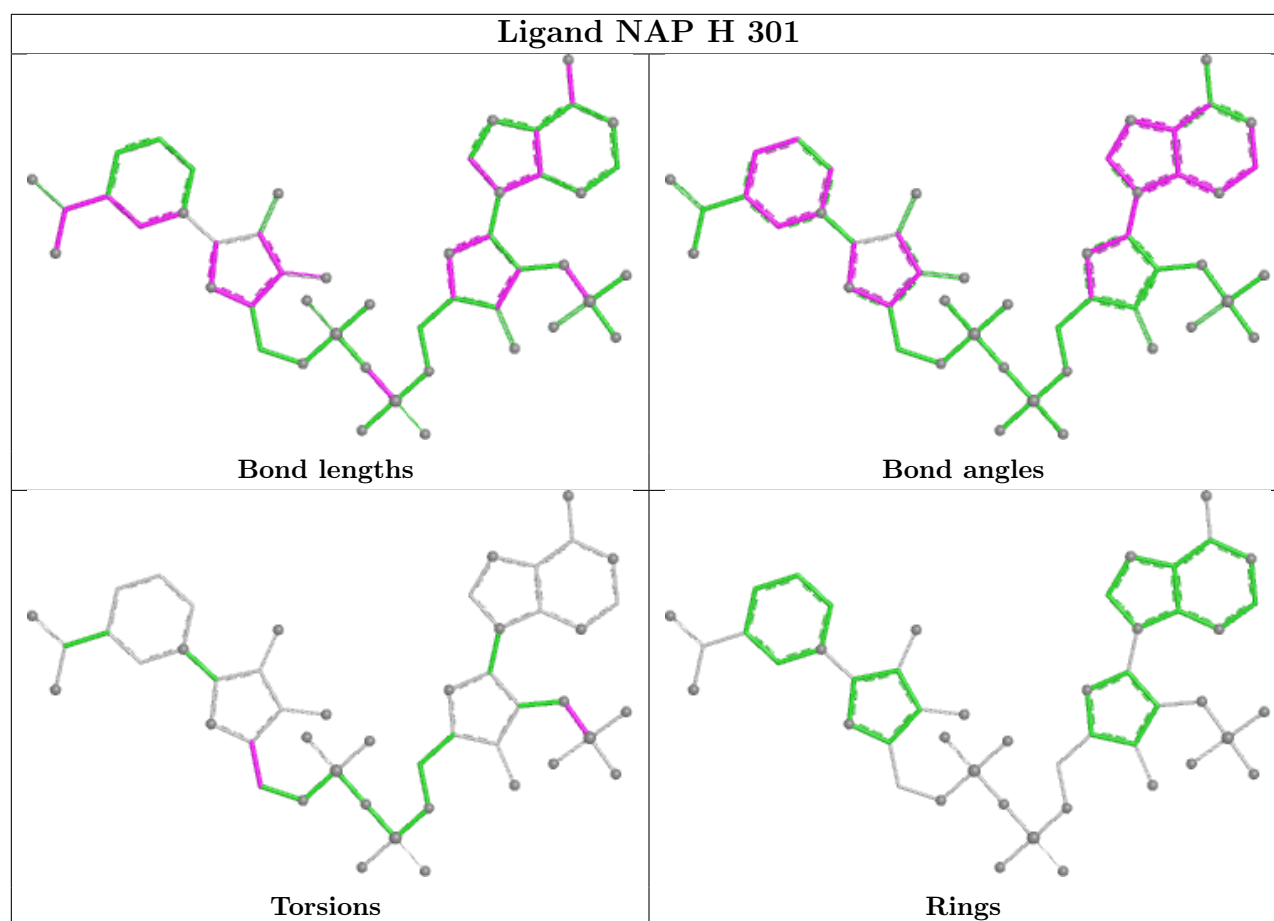












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	256/259 (98%)	0.15	19 (7%)	20 22	13, 26, 67, 97	0
1	B	255/259 (98%)	0.36	17 (6%)	24 25	18, 33, 67, 102	0
1	C	258/259 (99%)	0.12	10 (3%)	43 46	19, 32, 51, 81	0
1	D	259/259 (100%)	0.37	12 (4%)	37 40	18, 34, 50, 84	0
1	E	255/259 (98%)	0.10	10 (3%)	43 46	17, 31, 54, 67	0
1	F	254/259 (98%)	0.09	13 (5%)	33 36	16, 28, 56, 79	0
1	G	256/259 (98%)	0.34	9 (3%)	47 50	20, 35, 61, 71	0
1	H	253/259 (97%)	-0.00	3 (1%)	76 79	18, 30, 49, 63	0
1	I	258/259 (99%)	0.67	19 (7%)	20 22	27, 43, 67, 81	0
1	J	257/259 (99%)	0.77	12 (4%)	36 39	29, 44, 72, 105	0
1	K	255/259 (98%)	0.94	36 (14%)	6 6	27, 47, 79, 106	0
1	L	253/259 (97%)	0.65	21 (8%)	17 18	28, 41, 66, 82	0
1	M	256/259 (98%)	0.88	31 (12%)	8 9	27, 45, 81, 110	0
1	N	254/259 (98%)	0.79	19 (7%)	20 21	29, 47, 67, 79	0
1	O	253/259 (97%)	0.65	6 (2%)	59 63	30, 45, 64, 76	0
1	P	255/259 (98%)	0.79	19 (7%)	20 21	29, 42, 67, 93	0
All	All	4087/4144 (98%)	0.48	256 (6%)	26 27	13, 38, 66, 110	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	254	LEU	9.6
1	D	255	ALA	8.9
1	B	203	LEU	8.4
1	A	203	LEU	7.5
1	M	203	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
1	C	254	LEU	7.2
1	J	254	LEU	6.5
1	J	255	ALA	6.2
1	B	195	LEU	6.1
1	B	194	GLY	6.0
1	J	256	ILE	5.9
1	K	203	LEU	5.9
1	G	203	LEU	5.6
1	D	256	ILE	5.6
1	P	203	LEU	5.4
1	F	203	LEU	5.4
1	A	205	GLN	5.3
1	C	256	ILE	5.2
1	A	194	GLY	5.2
1	M	194	GLY	5.1
1	M	195	LEU	5.0
1	K	205	GLN	5.0
1	B	202	TYR	5.0
1	C	255	ALA	4.9
1	C	253	HIS	4.9
1	M	206	MET	4.9
1	D	257	ALA	4.8
1	B	204	ASP	4.7
1	B	254	LEU	4.5
1	B	198	MET	4.4
1	M	205	GLN	4.4
1	A	89	CYS	4.4
1	K	128	GLN	4.3
1	J	253	HIS	4.3
1	I	254	LEU	4.2
1	M	198	MET	4.2
1	I	256	ILE	4.1
1	A	254	LEU	4.1
1	P	-1	SER	3.9
1	B	205	GLN	3.9
1	K	112	LEU	3.9
1	C	179	LYS	3.9
1	F	253	HIS	3.9
1	I	255	ALA	3.8
1	P	253	HIS	3.8
1	G	254	LEU	3.8
1	M	202	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	257	ALA	3.7
1	N	179	LYS	3.7
1	A	195	LEU	3.6
1	K	204	ASP	3.6
1	J	1	MET	3.6
1	K	202	TYR	3.6
1	K	206	MET	3.6
1	O	253	HIS	3.5
1	L	203	LEU	3.5
1	A	202	TYR	3.5
1	A	204	ASP	3.5
1	P	202	TYR	3.4
1	L	52	SER	3.4
1	N	178	LYS	3.3
1	B	196	ASP	3.3
1	D	55	ARG	3.3
1	M	191	MET	3.2
1	O	252	SER	3.2
1	M	47	THR	3.1
1	A	198	MET	3.1
1	L	195	LEU	3.1
1	N	0	HIS	3.1
1	I	194	GLY	3.1
1	M	254	LEU	3.1
1	A	196	ASP	3.1
1	K	-1	SER	3.1
1	I	253	HIS	3.1
1	J	128	GLN	3.0
1	B	206	MET	3.0
1	D	253	HIS	3.0
1	H	0	HIS	3.0
1	I	0	HIS	3.0
1	A	-1	SER	3.0
1	A	207	ALA	3.0
1	M	1	MET	3.0
1	E	253	HIS	3.0
1	L	55	ARG	3.0
1	G	253	HIS	2.9
1	J	0	HIS	2.9
1	F	194	GLY	2.9
1	K	194	GLY	2.9
1	F	206	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	253	HIS	2.9
1	B	0	HIS	2.9
1	L	196	ASP	2.9
1	M	199	GLY	2.9
1	M	204	ASP	2.9
1	D	0	HIS	2.9
1	J	2	PHE	2.9
1	I	191	MET	2.9
1	K	253	HIS	2.8
1	C	-1	SER	2.8
1	P	205	GLN	2.8
1	E	195	LEU	2.8
1	M	253	HIS	2.8
1	K	207	ALA	2.8
1	M	2	PHE	2.8
1	G	39	ARG	2.8
1	K	195	LEU	2.8
1	N	199	GLY	2.7
1	K	192	THR	2.7
1	H	191	MET	2.7
1	M	16	SER	2.7
1	M	207	ALA	2.7
1	N	203	LEU	2.7
1	G	0	HIS	2.7
1	I	84	GLY	2.7
1	N	191	MET	2.7
1	O	52	SER	2.7
1	L	1	MET	2.6
1	A	193	GLU	2.6
1	M	0	HIS	2.6
1	L	191	MET	2.6
1	F	196	ASP	2.6
1	L	53	GLY	2.6
1	K	125	ALA	2.6
1	M	192	THR	2.6
1	P	80	SER	2.6
1	K	191	MET	2.6
1	M	128	GLN	2.6
1	N	134	GLY	2.6
1	K	24	ALA	2.6
1	M	196	ASP	2.5
1	L	194	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	87	ILE	2.5
1	J	252	SER	2.5
1	F	205	GLN	2.5
1	B	69	GLU	2.5
1	L	197	GLU	2.5
1	I	100	LEU	2.5
1	I	127	LEU	2.5
1	K	0	HIS	2.5
1	L	49	ALA	2.5
1	P	128	GLN	2.5
1	A	206	MET	2.5
1	F	195	LEU	2.5
1	N	2	PHE	2.5
1	P	199	GLY	2.5
1	N	253	HIS	2.5
1	F	198	MET	2.5
1	E	35	VAL	2.5
1	N	177	PRO	2.5
1	K	62	ARG	2.4
1	E	203	LEU	2.4
1	M	215	LEU	2.4
1	B	197	GLU	2.4
1	I	197	GLU	2.4
1	K	80	SER	2.4
1	F	207	ALA	2.4
1	N	76	ALA	2.4
1	L	128	GLN	2.4
1	D	83	GLY	2.4
1	N	1	MET	2.4
1	E	191	MET	2.4
1	H	1	MET	2.4
1	K	196	ASP	2.3
1	C	0	HIS	2.3
1	G	194	GLY	2.3
1	K	199	GLY	2.3
1	N	53	GLY	2.3
1	P	204	ASP	2.3
1	J	76	ALA	2.3
1	D	-1	SER	2.3
1	N	46	ARG	2.3
1	G	196	ASP	2.3
1	K	61	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	203	LEU	2.3
1	K	127	LEU	2.3
1	L	74	THR	2.3
1	P	191	MET	2.3
1	E	53	GLY	2.3
1	N	48	VAL	2.3
1	J	191	MET	2.3
1	L	17	LYS	2.3
1	K	197	GLU	2.2
1	M	28	ALA	2.2
1	I	179	LYS	2.2
1	N	131	THR	2.2
1	K	193	GLU	2.2
1	L	103	LEU	2.2
1	M	197	GLU	2.2
1	A	200	GLN	2.2
1	A	208	SER	2.2
1	E	-1	SER	2.2
1	J	204	ASP	2.2
1	M	200	GLN	2.2
1	N	84	GLY	2.2
1	P	194	GLY	2.2
1	K	219	ALA	2.2
1	L	0	HIS	2.2
1	K	198	MET	2.2
1	B	37	THR	2.2
1	B	200	GLN	2.2
1	E	128	GLN	2.2
1	F	201	ASP	2.2
1	M	252	SER	2.2
1	N	196	ASP	2.2
1	L	209	ALA	2.2
1	F	191	MET	2.2
1	A	197	GLU	2.2
1	K	46	ARG	2.2
1	C	1	MET	2.1
1	I	1	MET	2.1
1	K	151	TYR	2.1
1	P	122	ILE	2.1
1	I	196	ASP	2.1
1	P	59	THR	2.1
1	C	208	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	53	GLY	2.1
1	I	57	LYS	2.1
1	C	191	MET	2.1
1	I	204	ASP	2.1
1	B	62	ARG	2.1
1	G	58	VAL	2.1
1	P	0	HIS	2.1
1	O	168	LEU	2.1
1	P	127	LEU	2.1
1	P	126	ALA	2.1
1	M	95	PHE	2.1
1	K	201	ASP	2.1
1	L	202	TYR	2.1
1	L	204	ASP	2.1
1	M	190	ILE	2.1
1	O	191	MET	2.1
1	E	0	HIS	2.1
1	M	40	ASN	2.1
1	B	201	ASP	2.1
1	P	196	ASP	2.1
1	F	197	GLU	2.0
1	K	97	SER	2.0
1	M	-1	SER	2.0
1	E	202	TYR	2.0
1	D	1	MET	2.0
1	D	191	MET	2.0
1	L	78	THR	2.0
1	K	20	GLY	2.0
1	P	7	GLY	2.0
1	K	200	GLN	2.0
1	L	40	ASN	2.0
1	O	100	LEU	2.0
1	K	76	ALA	2.0
1	K	209	ALA	2.0
1	M	209	ALA	2.0
1	A	201	ASP	2.0
1	D	53	GLY	2.0
1	F	202	TYR	2.0
1	G	202	TYR	2.0
1	K	75	VAL	2.0
1	N	61	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	M	304	1/1	0.75	0.28	71,71,71,71	0
5	MG	F	304	1/1	0.79	0.12	52,52,52,52	0
3	F3V	M	302	5/5	0.79	0.21	66,68,68,68	0
5	MG	J	304	1/1	0.85	0.10	42,42,42,42	0
5	MG	C	304	1/1	0.88	0.09	24,24,24,24	0
4	CL	A	304	1/1	0.88	0.18	82,82,82,82	0
2	NAP	M	301	48/48	0.89	0.14	42,53,62,63	48
3	F3V	I	302	5/5	0.89	0.13	44,44,47,48	0
5	MG	L	304	1/1	0.90	0.09	66,66,66,66	0
3	F3V	E	302	5/5	0.91	0.10	25,27,31,33	0
3	F3V	P	302	5/5	0.91	0.16	45,47,49,50	0
3	F3V	G	302	5/5	0.91	0.12	39,39,40,41	0
2	NAP	B	301	48/48	0.91	0.12	24,32,41,42	48
3	F3V	N	302	5/5	0.92	0.13	42,43,44,45	0
3	F3V	J	302	5/5	0.92	0.12	43,45,45,46	0
3	F3V	K	302	5/5	0.92	0.12	45,46,48,50	0
2	NAP	K	301	48/48	0.92	0.11	35,38,42,44	48
4	CL	M	303	1/1	0.93	0.21	53,53,53,53	0
3	F3V	L	302	5/5	0.93	0.11	47,50,52,53	0
2	NAP	G	301	48/48	0.93	0.10	19,27,32,32	48
5	MG	H	304	1/1	0.93	0.09	28,28,28,28	0
2	NAP	N	301	48/48	0.93	0.10	31,41,51,52	48
3	F3V	A	302	5/5	0.93	0.11	35,36,37,37	0
2	NAP	L	301	48/48	0.93	0.10	32,45,49,51	0
2	NAP	E	301	48/48	0.94	0.09	20,27,32,34	48
2	NAP	F	301	48/48	0.94	0.09	17,32,38,41	48
3	F3V	F	302	5/5	0.94	0.09	35,39,41,42	0

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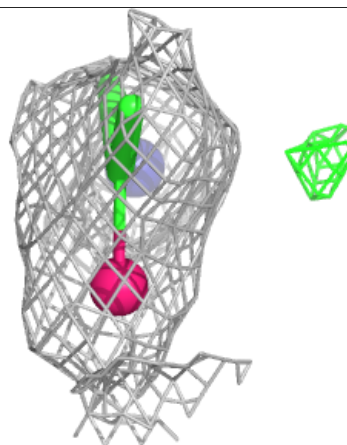
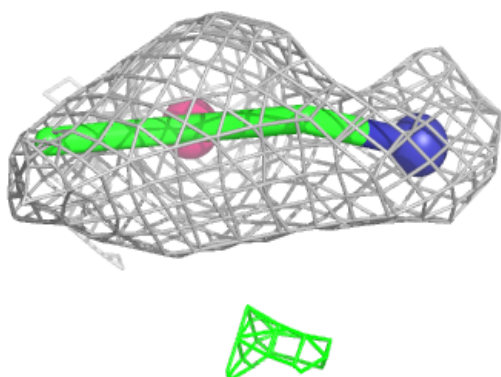
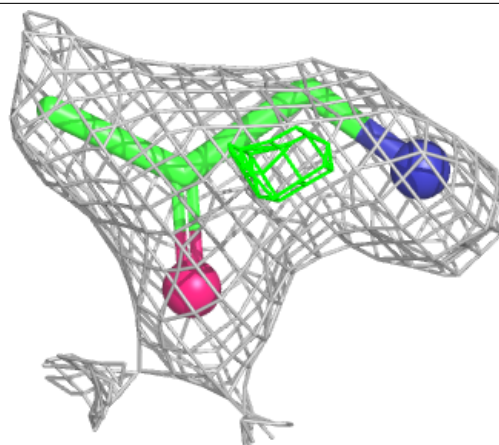
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	A	301	48/48	0.94	0.09	16,29,34,36	48
3	F3V	O	302	5/5	0.94	0.09	35,35,39,40	0
2	NAP	I	301	48/48	0.94	0.09	31,37,43,46	48
2	NAP	P	301	48/48	0.94	0.09	32,35,41,45	48
5	MG	O	304	1/1	0.94	0.11	45,45,45,45	0
2	NAP	O	301	48/48	0.95	0.08	31,35,42,45	0
3	F3V	B	302	5/5	0.95	0.11	38,42,44,46	0
3	F3V	D	302	5/5	0.95	0.08	22,23,23,26	0
4	CL	J	303	1/1	0.95	0.14	56,56,56,56	0
2	NAP	D	301	48/48	0.95	0.08	17,22,27,30	0
4	CL	O	303	1/1	0.95	0.15	47,47,47,47	0
4	CL	P	303	1/1	0.95	0.11	49,49,49,49	0
2	NAP	J	301	48/48	0.96	0.07	28,34,36,38	0
2	NAP	H	301	48/48	0.96	0.06	12,18,24,25	0
2	NAP	C	301	48/48	0.96	0.07	12,19,25,32	0
5	MG	A	305	1/1	0.96	0.08	43,43,43,43	0
3	F3V	C	302	5/5	0.96	0.07	24,24,26,26	0
4	CL	B	303	1/1	0.96	0.12	37,37,37,37	0
4	CL	C	303	1/1	0.96	0.16	31,31,31,31	0
4	CL	I	303	1/1	0.96	0.14	65,65,65,65	0
3	F3V	H	302	5/5	0.96	0.07	23,24,24,26	0
4	CL	K	303	1/1	0.96	0.23	57,57,57,57	0
4	CL	L	303	1/1	0.96	0.19	52,52,52,52	0
4	CL	E	303	1/1	0.97	0.18	36,36,36,36	0
4	CL	F	303	1/1	0.97	0.14	33,33,33,33	0
4	CL	H	303	1/1	0.97	0.12	34,34,34,34	0
4	CL	A	303	1/1	0.97	0.14	31,31,31,31	0
4	CL	N	303	1/1	0.97	0.20	47,47,47,47	0
4	CL	G	303	1/1	0.98	0.14	33,33,33,33	0
4	CL	D	303	1/1	0.98	0.14	33,33,33,33	0

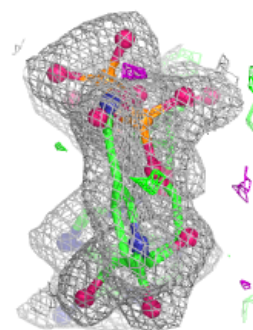
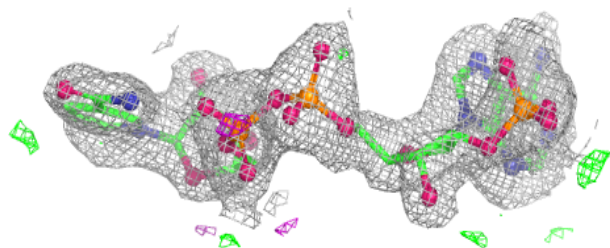
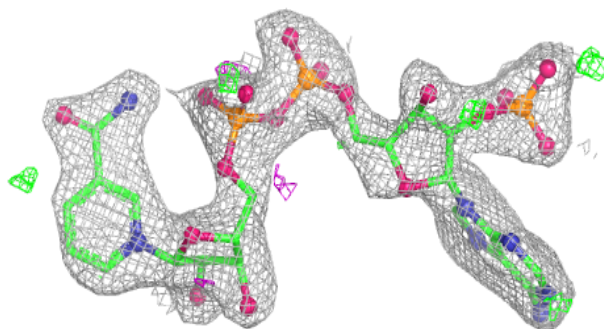
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F3V M 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

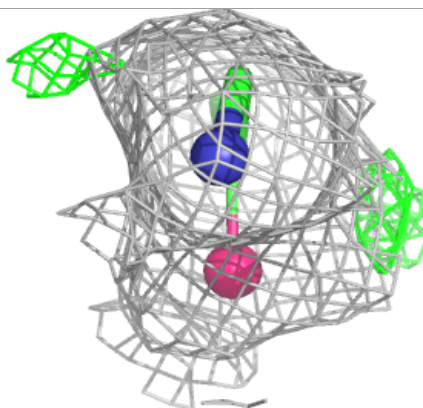
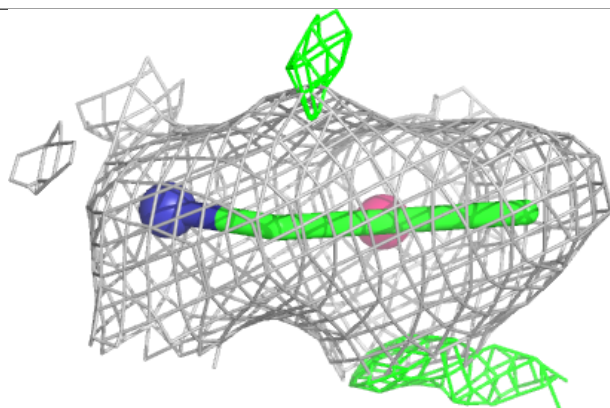
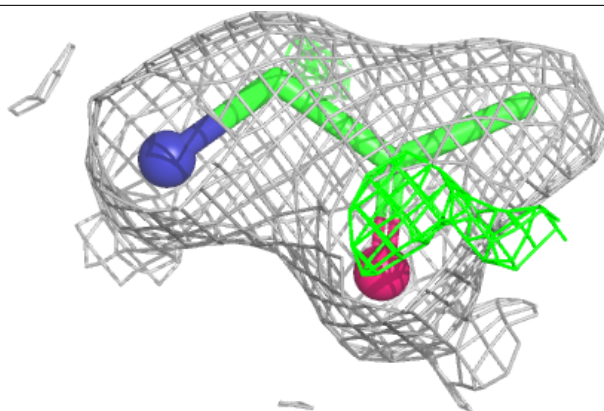
**Electron density around NAP M 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

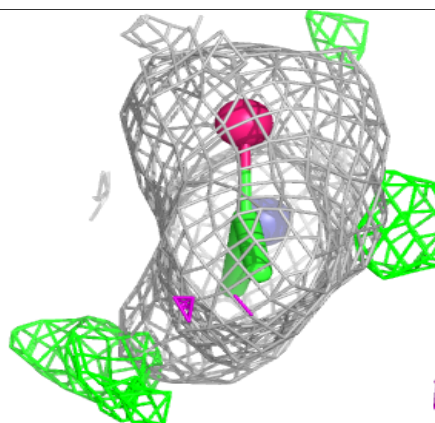
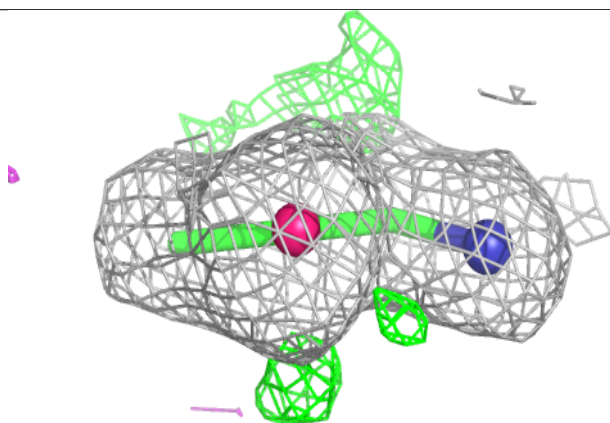
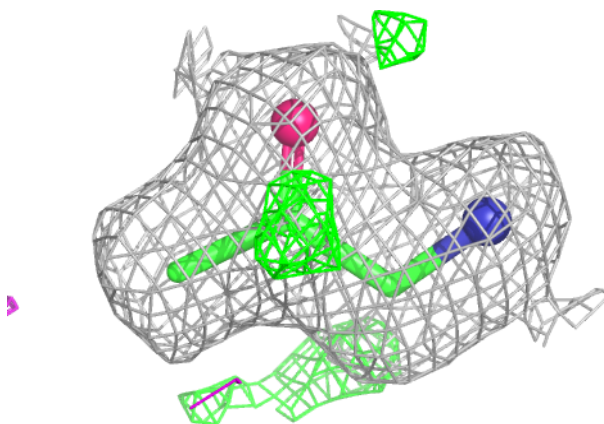


Electron density around F3V I 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

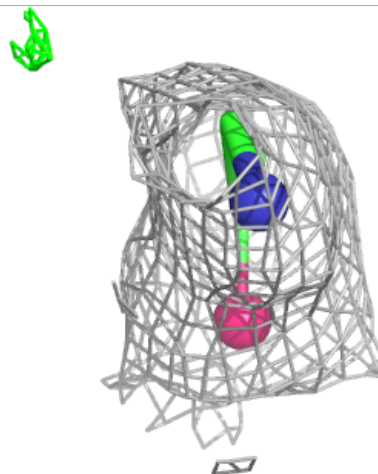
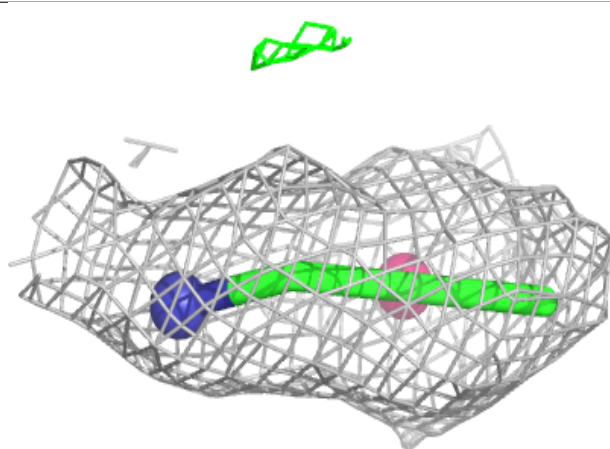
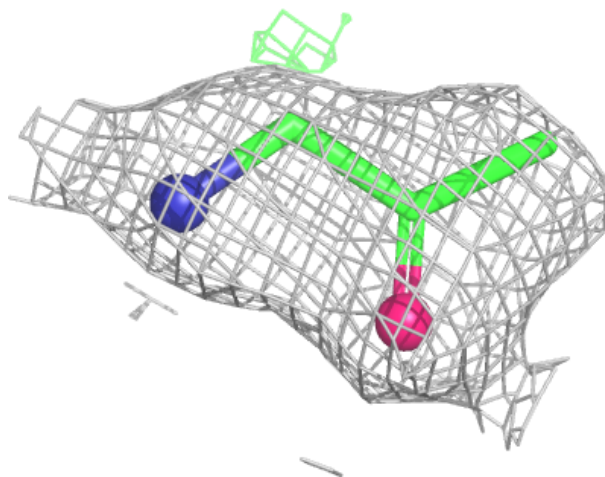
**Electron density around F3V E 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



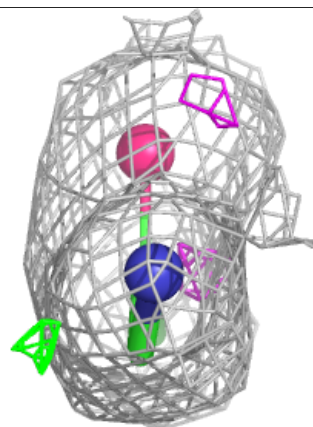
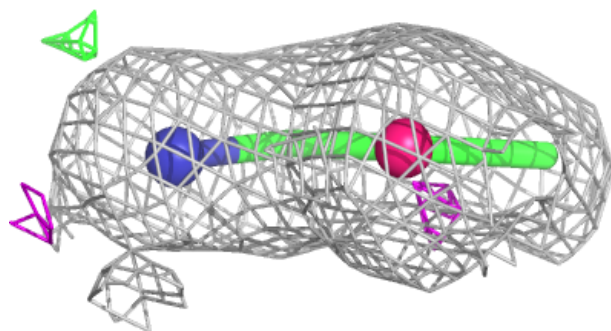
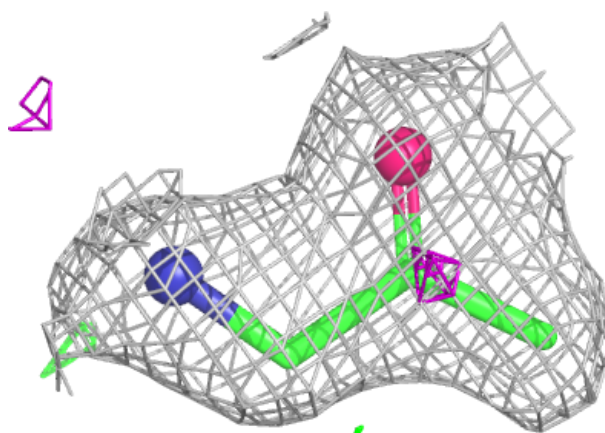
Electron density around F3V P 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

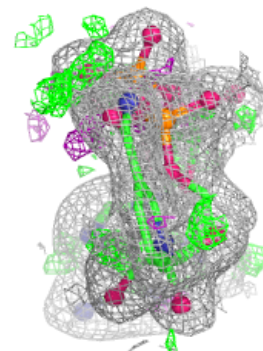
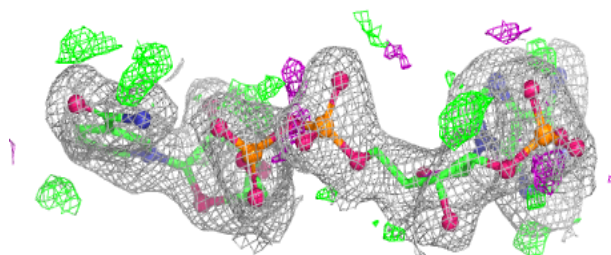
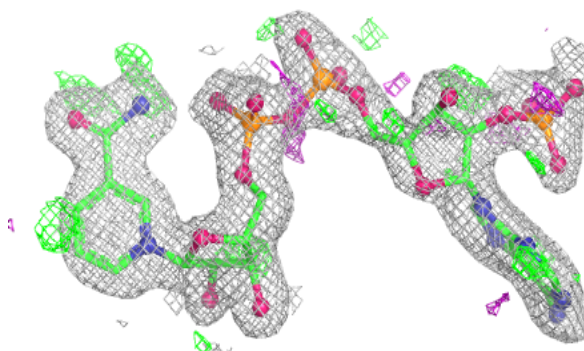


Electron density around F3V G 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

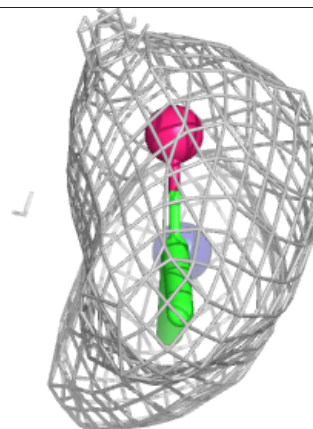
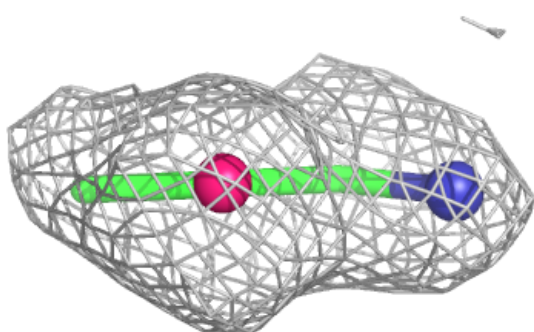
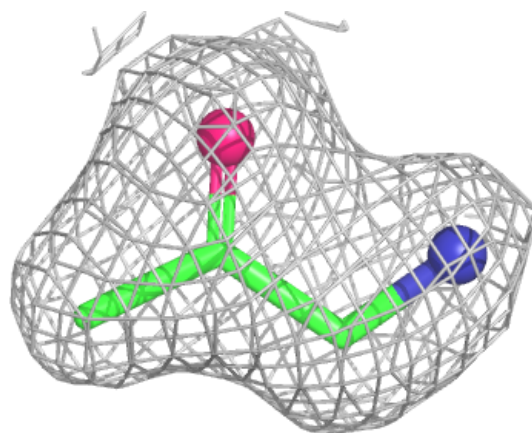
**Electron density around NAP B 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



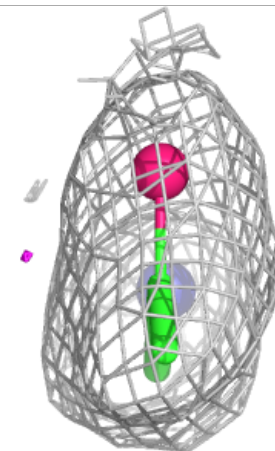
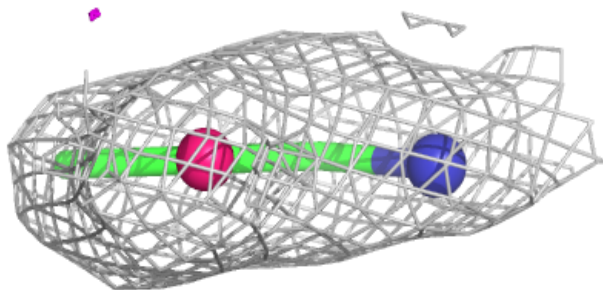
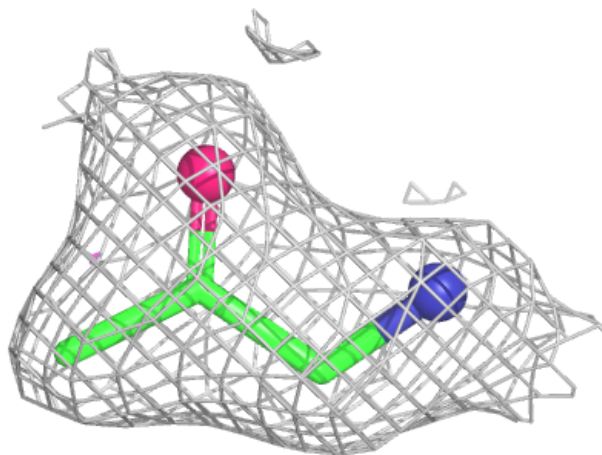
Electron density around F3V N 302:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



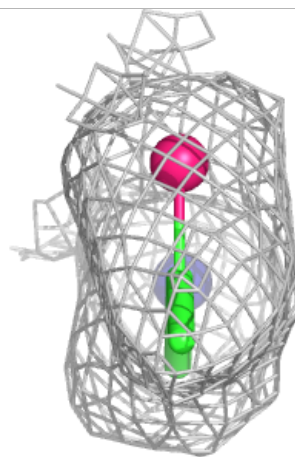
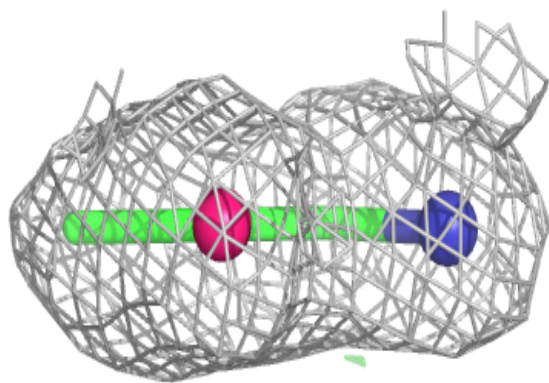
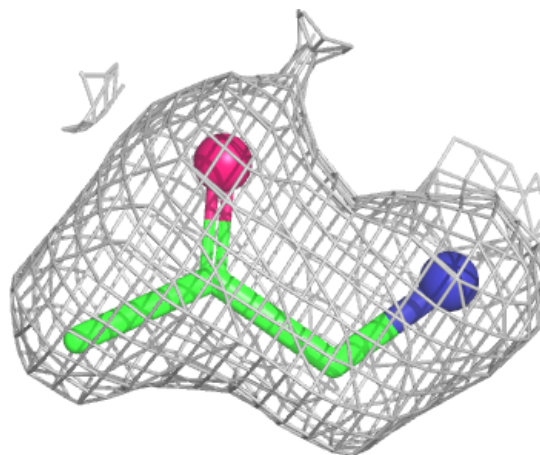
Electron density around F3V J 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



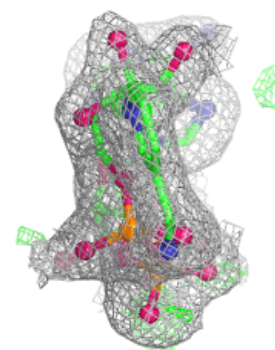
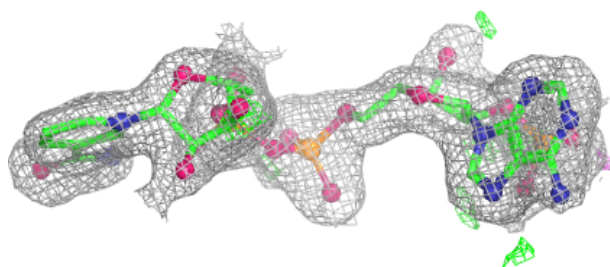
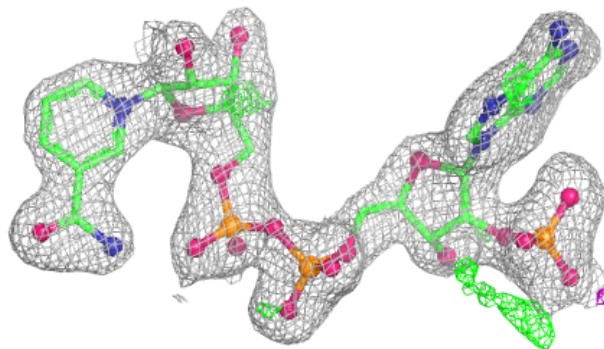
Electron density around F3V K 302:

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and green (positive)

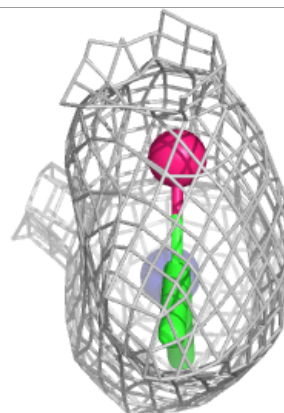
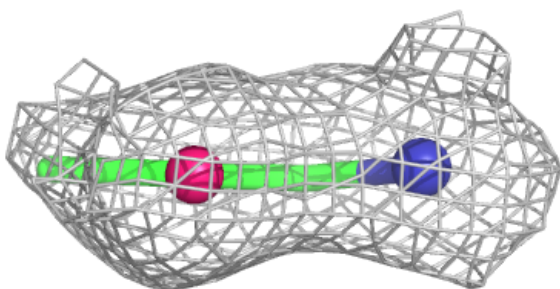
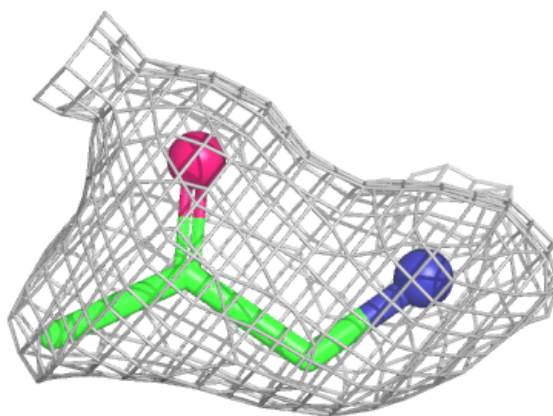


Electron density around NAP K 301:

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and green (positive)

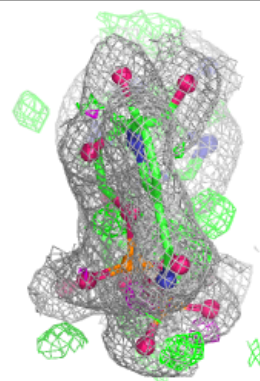
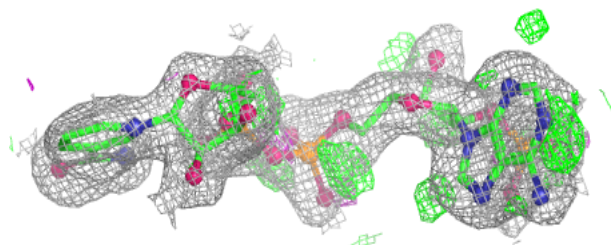
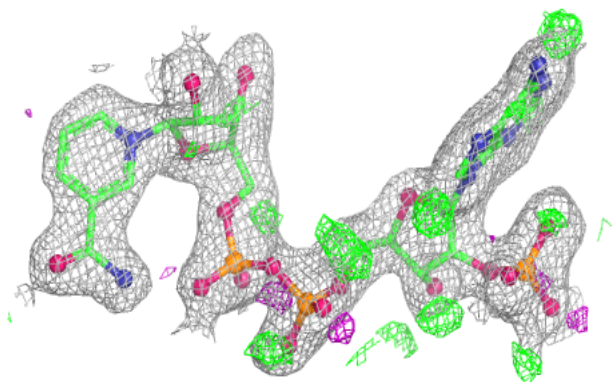
**Electron density around F3V L 302:**

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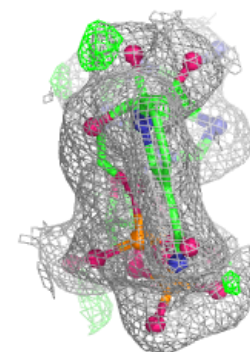
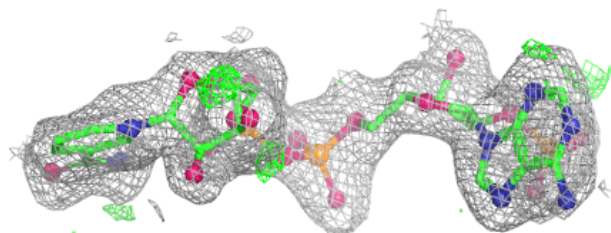
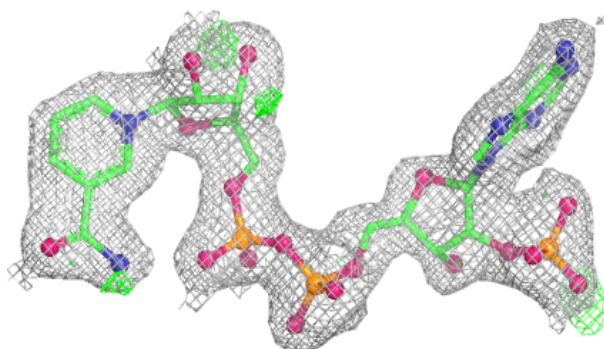


Electron density around NAP G 301:

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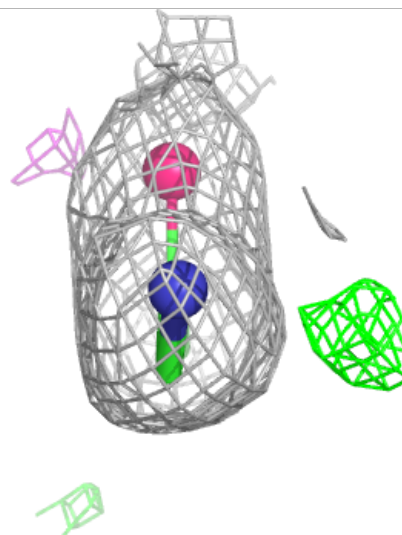
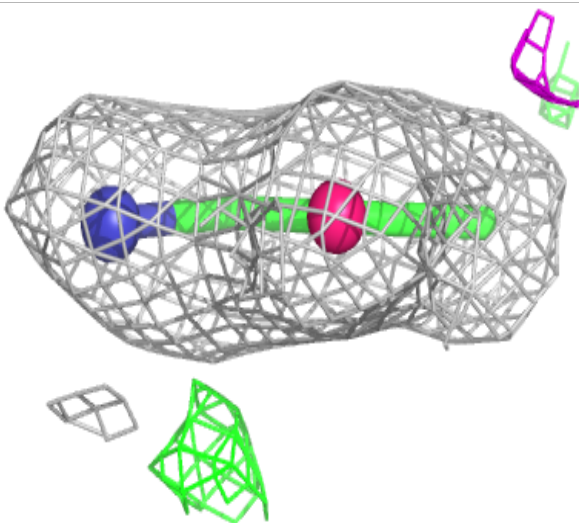
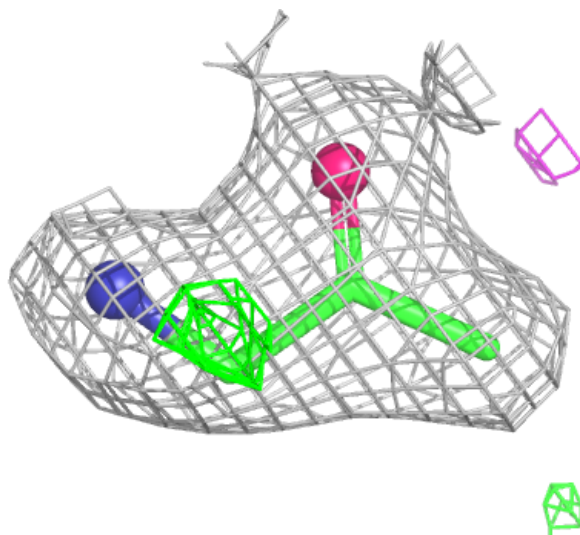
**Electron density around NAP N 301:**

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and green (positive)



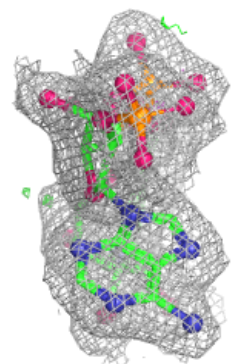
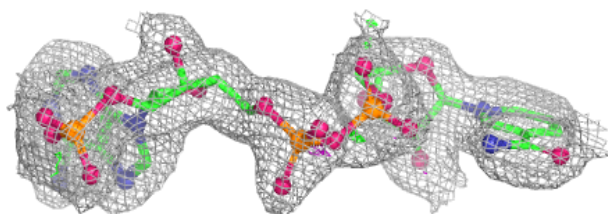
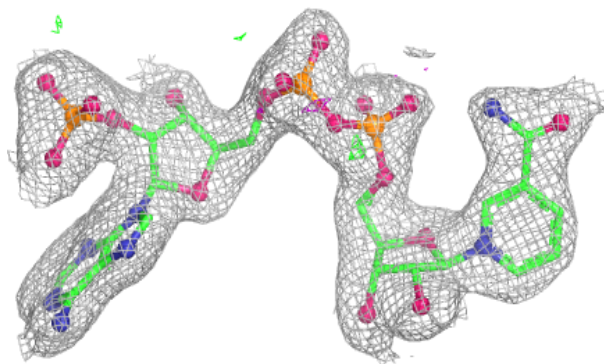
Electron density around F3V A 302:

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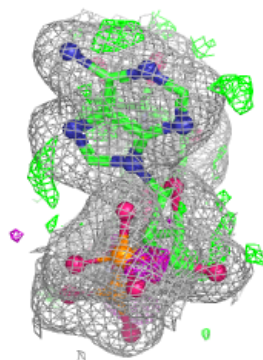
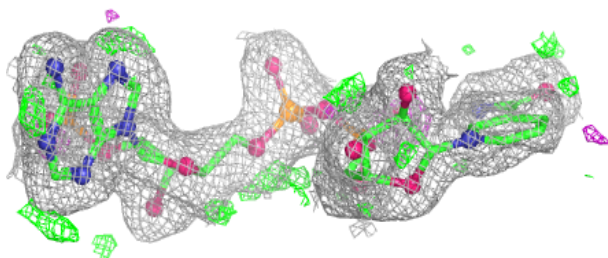
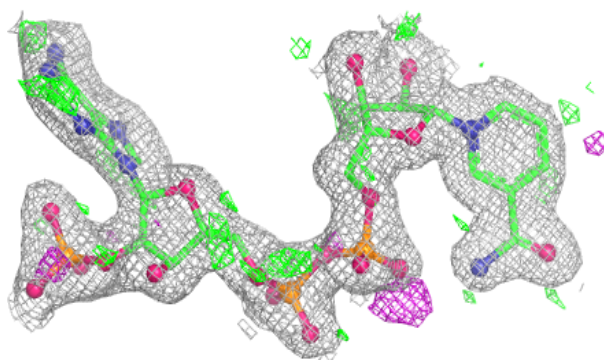


Electron density around NAP L 301:

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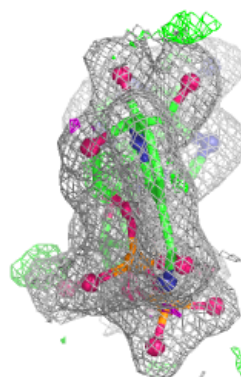
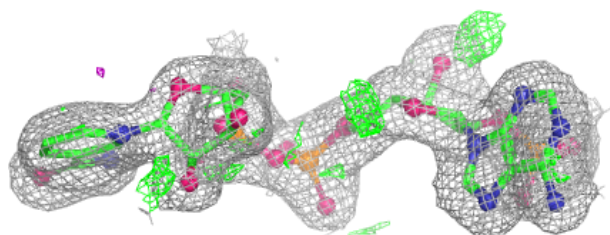
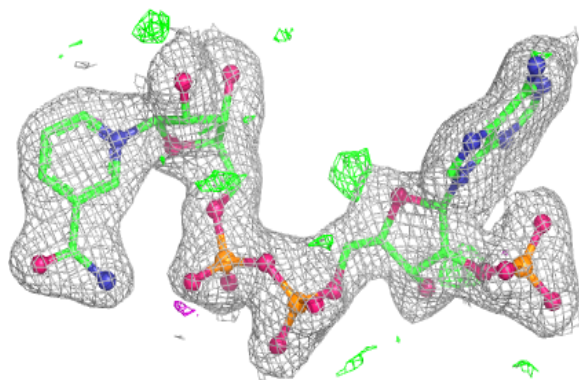
**Electron density around NAP E 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

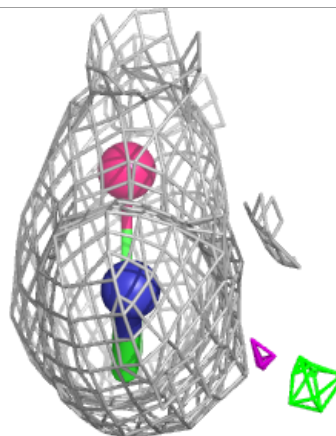
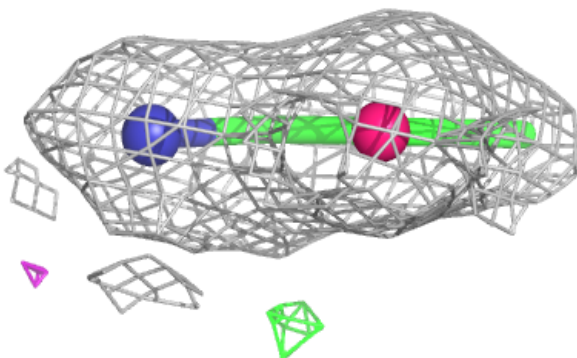
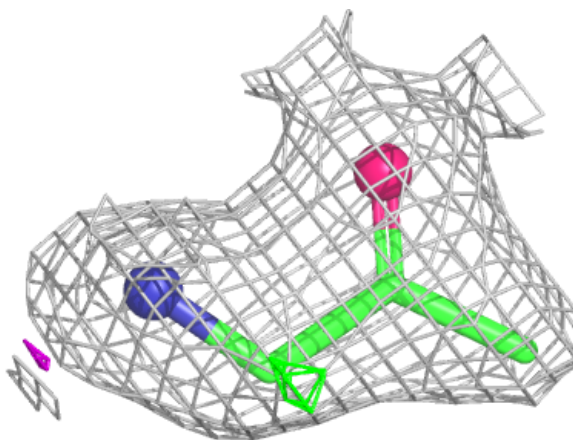


Electron density around NAP F 301:

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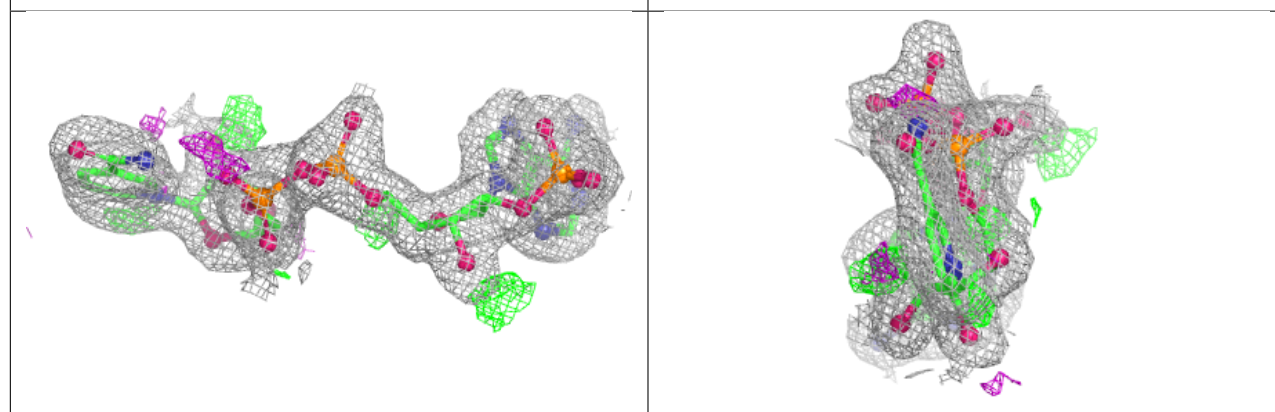
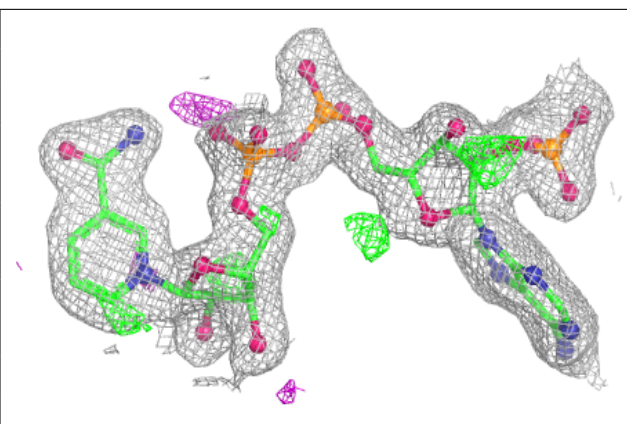
**Electron density around F3V F 302:**

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and green (positive)



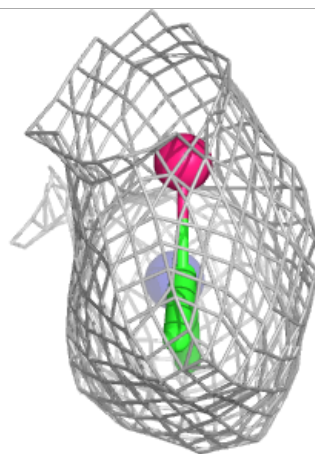
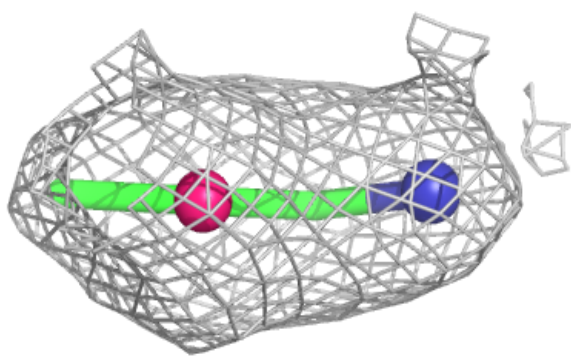
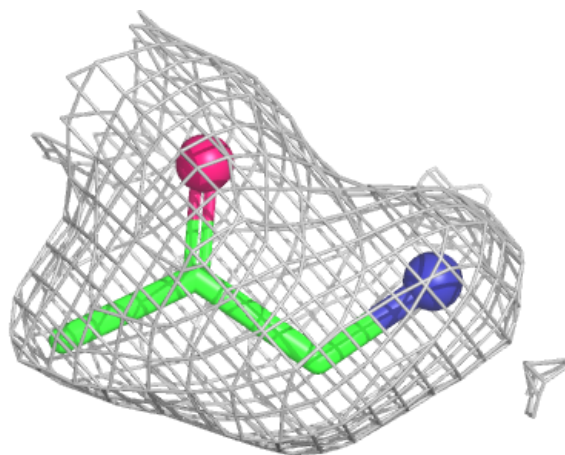
Electron density around NAP A 301:

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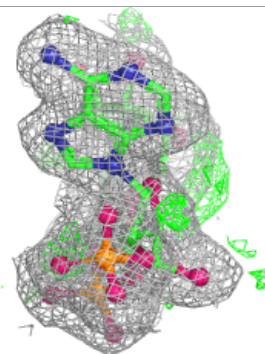
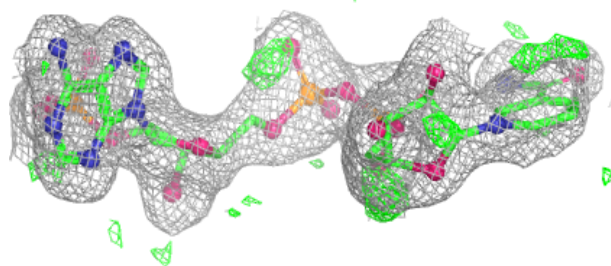
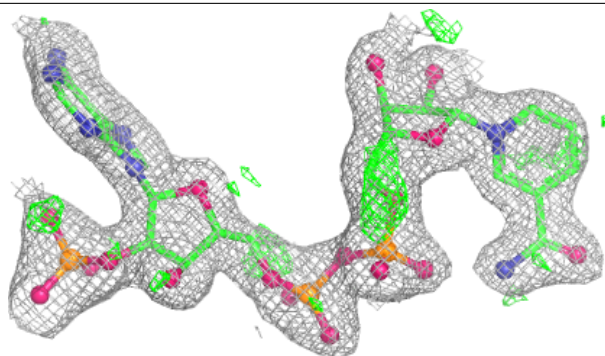
Electron density around F3V O 302:

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and green (positive)

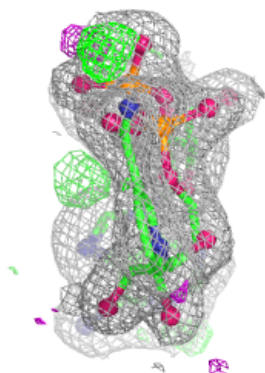
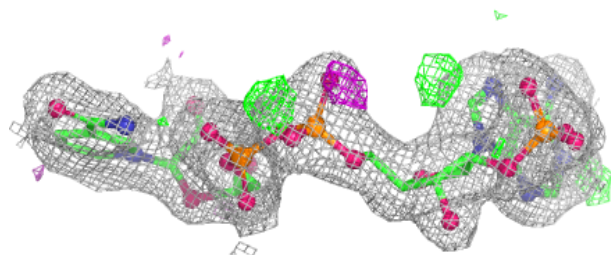
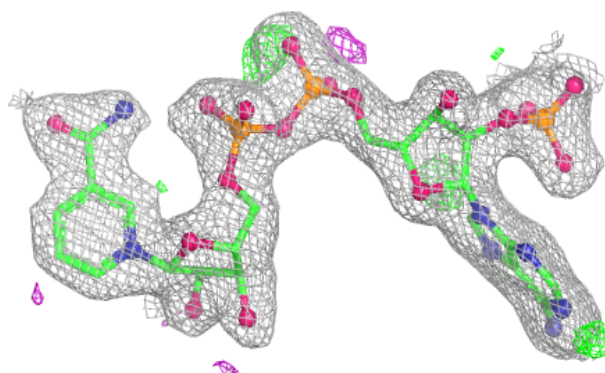


Electron density around NAP I 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

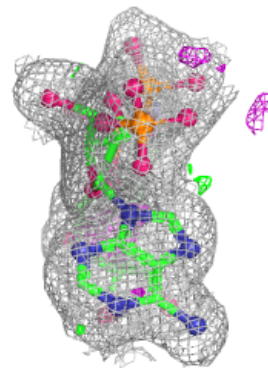
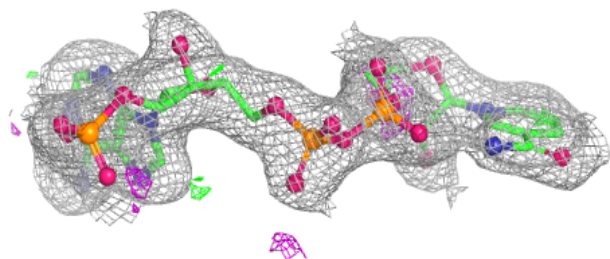
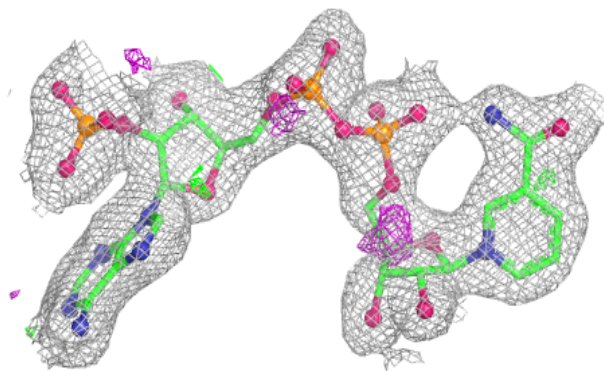
**Electron density around NAP P 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



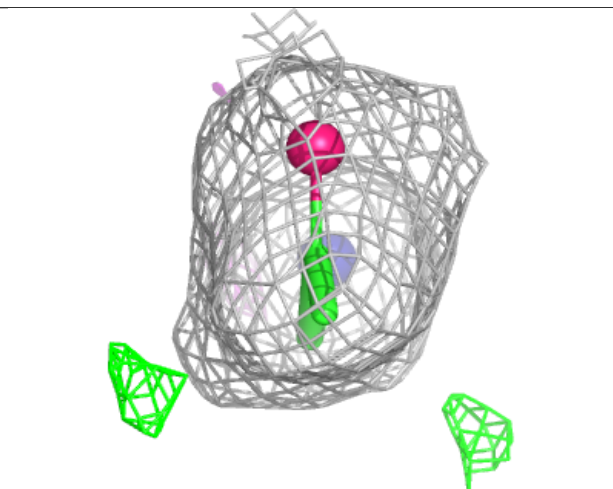
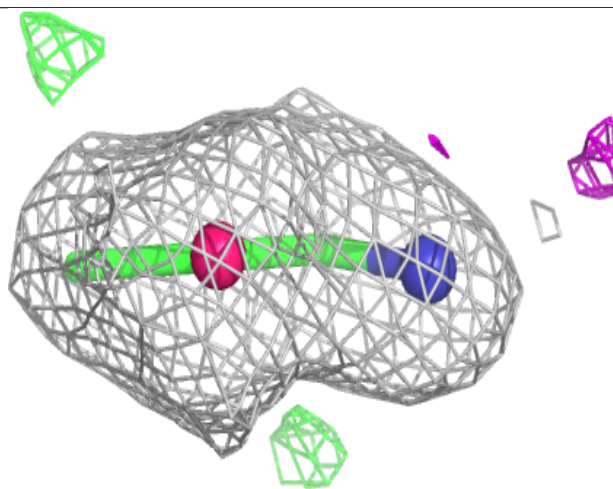
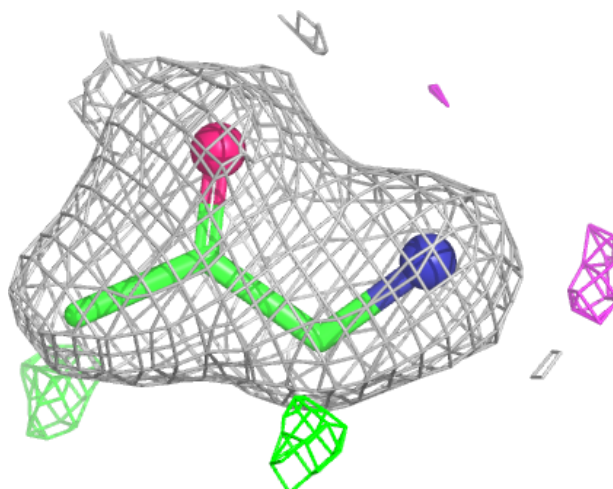
Electron density around NAP O 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



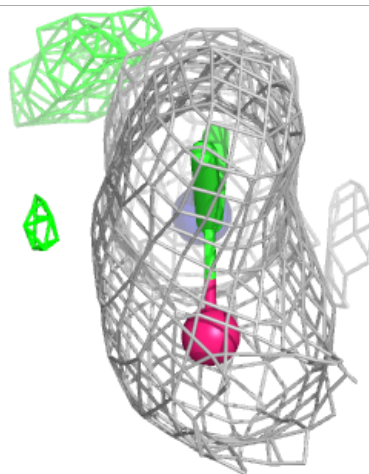
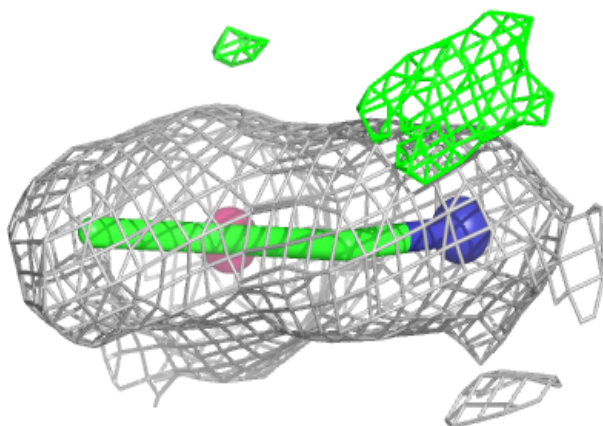
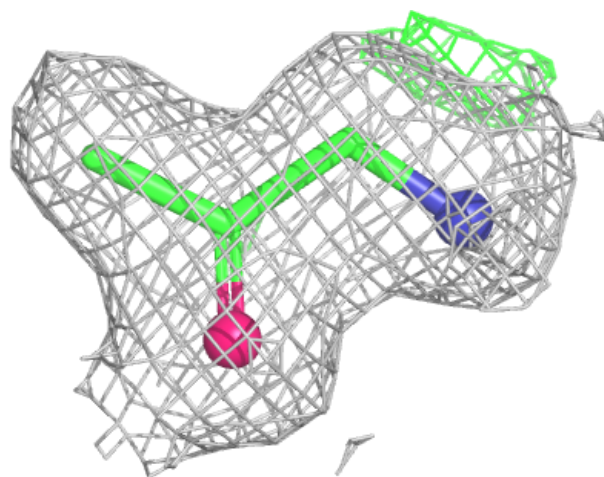
Electron density around F3V B 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



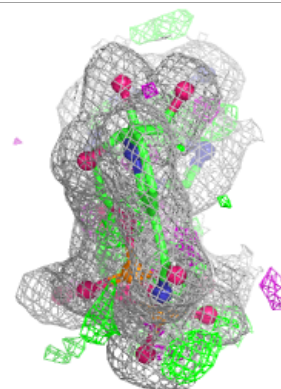
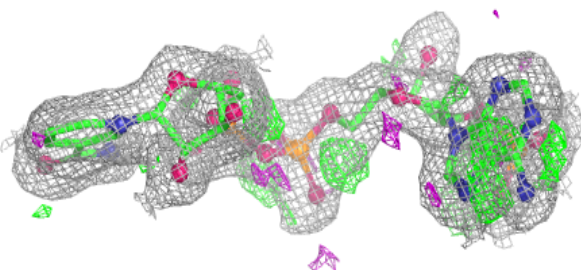
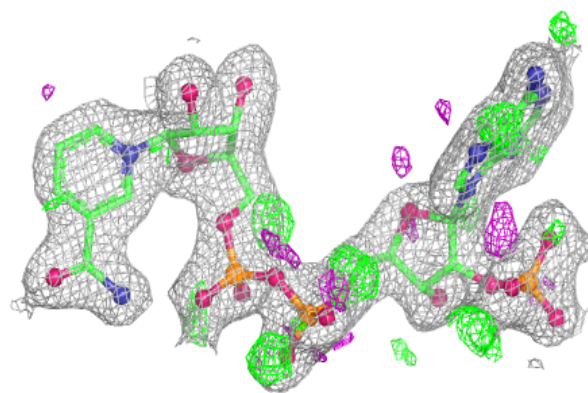
Electron density around F3V D 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

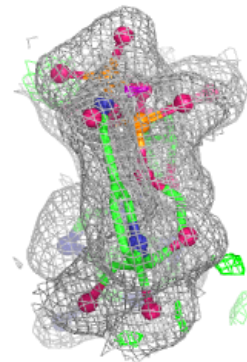
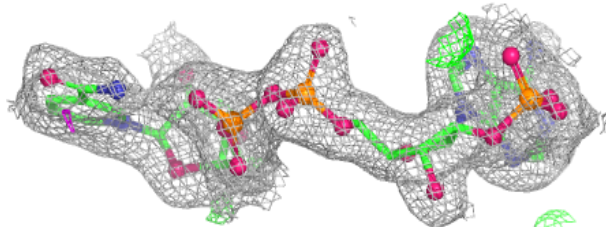
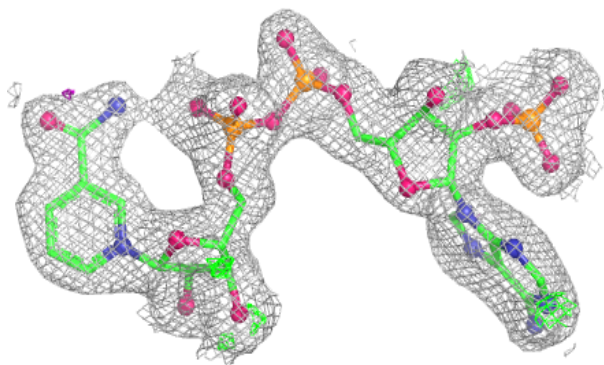


Electron density around NAP D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

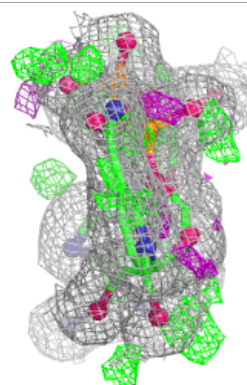
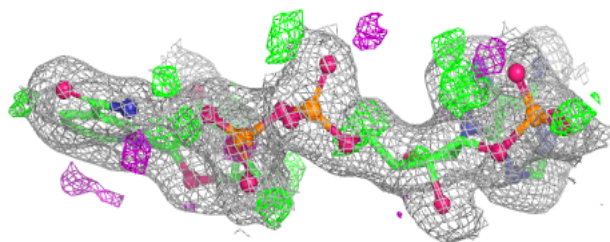
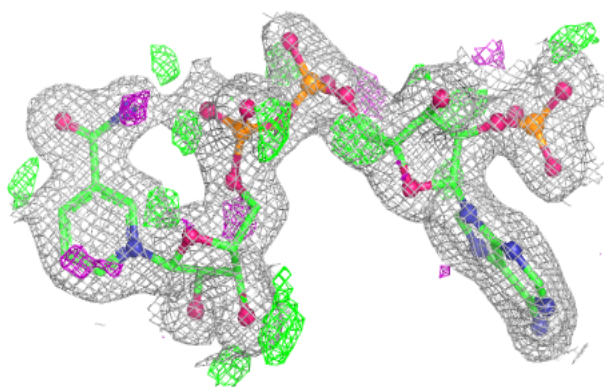
**Electron density around NAP J 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

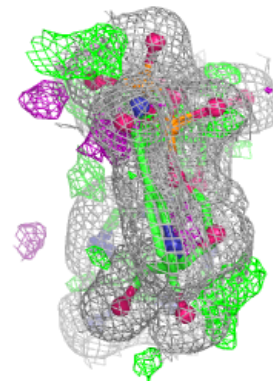
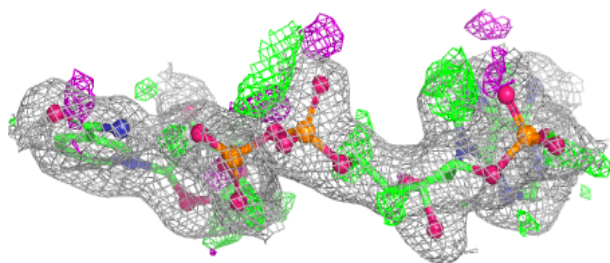
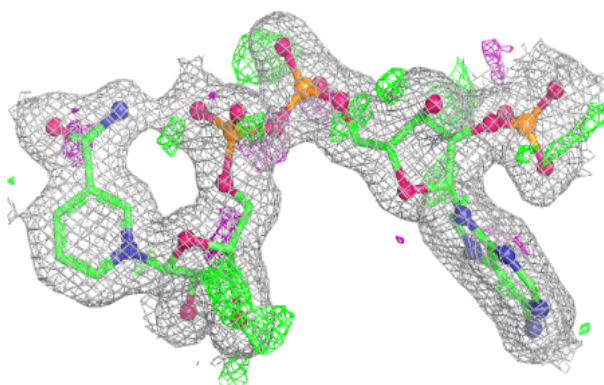


Electron density around NAP H 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

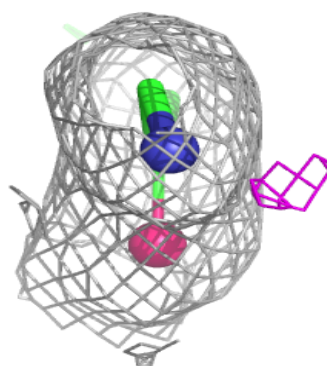
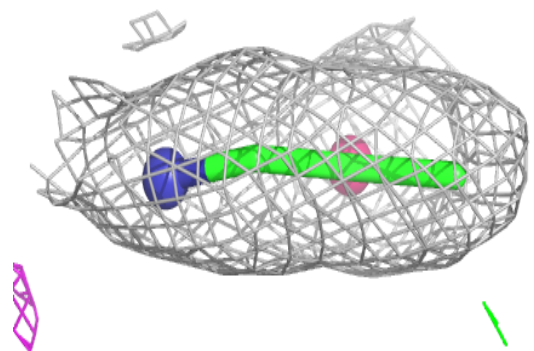
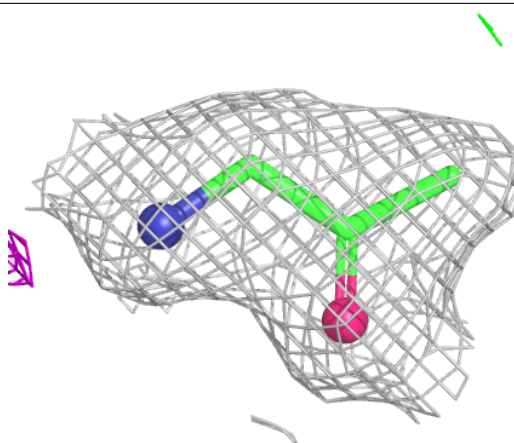
**Electron density around NAP C 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



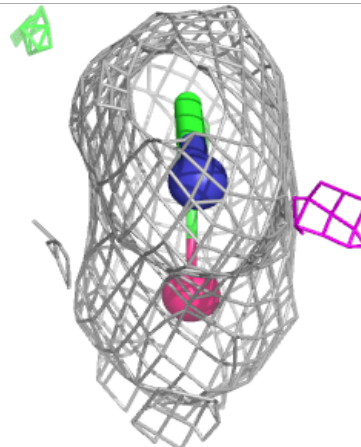
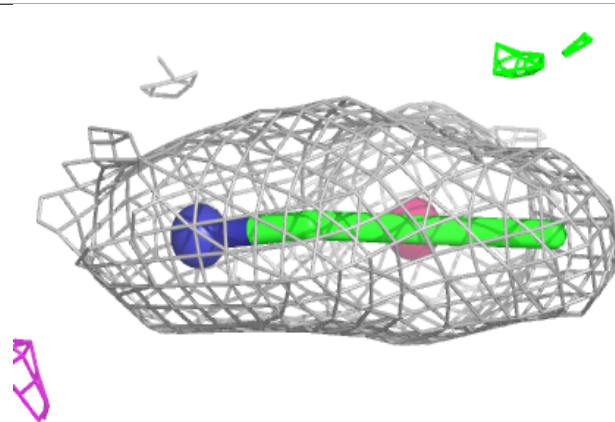
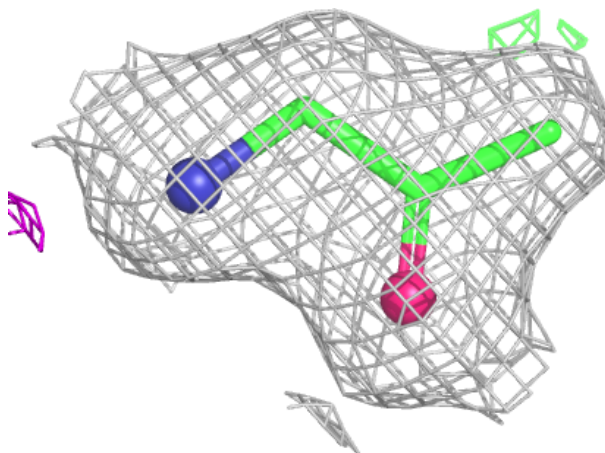
Electron density around F3V C 302:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around F3V H 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.